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TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS	3	OCT 07	EPFULL enhanced with full implementation of EPC2000
NEWS	4	OCT 07	Multiple databases enhanced for more flexible patent number searching
NEWS	5	OCT 22	Current-awareness alert (SDI) setup and editing enhanced
NEWS	6	OCT 22	WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT Applications
NEWS	7	OCT 24	CHEMLIST enhanced with intermediate list of pre-registered REACH substances
NEWS	8	NOV 21	CAS patent coverage to include exemplified prophetic substances identified in English-, French-, German-, and Japanese-language basic patents from 2004-present
NEWS	9	NOV 26	MARPAT enhanced with FSORT command
NEWS	10	NOV 26	MEDLINE year-end processing temporarily halts availability of new fully-indexed citations
NEWS	11	NOV 26	CHEMSAFE now available on STN Easy
NEWS	12	NOV 26	Two new SET commands increase convenience of STN searching
NEWS	13	DEC 01	ChemPort single article sales feature unavailable
NEWS	14	DEC 12	GBFULL now offers single source for full-text coverage of complete UK patent families
NEWS EXPRESS	JUNE 27 08	CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.	
NEWS HOURS	STN Operating Hours Plus Help Desk Availability		
NEWS LOGIN	Welcome Banner and News Items		
NEWS IPC8	For general information regarding STN implementation of IPC 8		

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 09:54:12 ON 16 DEC 2008

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 09:54:22 ON 16 DEC 2008
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STRUCTURE FILE UPDATES: 14 DEC 2008 HIGHEST RN 1084385-33-0
 DICTIONARY FILE UPDATES: 14 DEC 2008 HIGHEST RN 1084385-33-0

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<http://www.cas.org/support/stngen/stdoc/properties.html>

=> file caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.46	0.67

FILE 'CAPLUS' ENTERED AT 09:54:37 ON 16 DEC 2008
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FILE COVERS 1907 - 16 Dec 2008 VOL 149 ISS 25
 FILE LAST UPDATED: 15 Dec 2008 (20081215/ED)

Caplus now includes complete International Patent Classification (IPC)
 reclassification data for the third quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply.
 They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> s L1 SSS full

L1 NOT FOUND

The L-number entered has not been defined in this session, or it has been deleted. To see the L-numbers currently defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>).

=> d his

(FILE 'HOME' ENTERED AT 09:54:12 ON 16 DEC 2008)

FILE 'REGISTRY' ENTERED AT 09:54:22 ON 16 DEC 2008

FILE 'CAPLUS' ENTERED AT 09:54:37 ON 16 DEC 2008

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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1.15

FILE 'REGISTRY' ENTERED AT 09:54:52 ON 16 DEC 2008

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STRUCTURE FILE UPDATES: 14 DEC 2008 HIGHEST RN 1084385-33-0

DICTIONARY FILE UPDATES: 14 DEC 2008 HIGHEST RN 1084385-33-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\STNEXP\Queries\10579825 H or CH3.str



```

chain nodes :
6 13 14 15 16 18 19 20 21 22 23
ring nodes :
1 2 3 4 5 7 8 9 10 11 12
chain bonds :
1-6 2-13 4-7 13-14 13-16 14-15 18-19 18-20 21-22 21-23
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 1-5 1-6 13-14 13-16
exact bonds :
2-3 2-13 3-4 4-5 4-7 14-15 18-19 18-20 21-22 21-23
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 1 : 7 :

```

G1:O,S,N, [*1], [*2]

G2:H,CH3

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS
22:CLASS 23:CLASS

```

L1 STRUCTURE UPLOADED

=> d L1

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.46	1.61

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 09:55:11 ON 16 DEC 2008
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FILE COVERS 1907 - 16 Dec 2008 VOL 149 ISS 25
FILE LAST UPDATED: 15 Dec 2008 (20081215/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> s l1 SSS full
REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 09:55:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 11696 TO ITERATE

100.0% PROCESSED 11696 ITERATIONS 127 ANSWERS
SEARCH TIME: 00.00.01

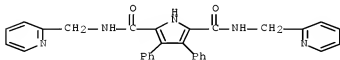
L2 127 SEA SSS FUL L1

L3 43 L2

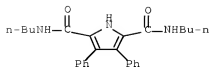
=> d ibib abs hitstr l-
YOU HAVE REQUESTED DATA FROM 43 ANSWERS - CONTINUE? Y/(N):y

L3 ANSWER 1 OF 43 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2008:908277 CAPLUS Full-text
 DOCUMENT NUMBER: 149:369113
 TITLE: Structural diversity in the first metal complexes of
 2,5-dicarboxamidopyrroles and
 2,5-dicarbothioamidopyrroles
 AUTHOR(S): Bates, Gareth W.; Gale, Philip A.; Light, Mark E.;
 Ogden, Mark I.; Warriner, Colin N.
 CORPORATE SOURCE: School of Chemistry, University of Southampton,
 Southampton, SO17 1BJ, UK
 SOURCE: Dalton Transactions (2008), (31), 4106-4112
 CODEN: DTARAF; ISSN: 1477-9226
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Metal complexes of 2,5-dicarboxamidopyrroles and 2,5-dicarbothioamidopyrroles
 were structurally characterized for the first time, complementing the
 significant amount of work that is reported for the analogous pyridine
 ligands. N,N'-Bis(3,5-dinitrophenyl)-3,4-diphenyl-1H-pyrrole-2,5-
 dicarboxamide forms octahedral bis(tridentate) complexes with Co(III) and
 Ni(II), where the ligands are bound to the metal centers through deprotonated
 pyrrole and amide N atoms. N,N'-Dibutyl-3,4-diphenyl-1H-pyrrole-2,5-
 dicarboxthioamide and N,N'-diphenyl-3,4-diphenyl-1H-pyrrole-2,5-
 dicarboxthioamide also form bis(tridentate) Co complexes, but are only
 deprotonated at the pyrrole N atom, the remainder of the coordination sphere
 comprising the thioamide S atoms. The di-Bu derivative was isolated as a
 Co(II) complex, whereas the di-Ph system deposited a Co(III) complex. In
 contrast, N,N'-dibutyl-3,4-dichloro-1H-pyrrole-2,5-dicarboxamide was found to
 act as a bidentate ligand in an octahedral Co(II) complex comprising two
 bidentate pyrrole ligands and two aqua ligands. Synthesis of N,N-bis(pyridin-
 2-ylmethyl)-3,4-diphenyl-1H-pyrrole-2,5-carboxamide gave a pyrrole ligand with
 increased denticity. Reaction with cobalt(II) chloride gave a dinuclear
 helicate complex. The ligand had undergone addition of a methoxy group to one
 of the linking methylene carbons, presumably as a result of the oxidative
 addition of solvent MeOH.
 IT 1056152-04-7P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (crystal structure; preparation of cobalt and nickel complexes of
 dicarboxamidopyrrole and dicarbothioamidopyrrole)
 RN 1058152-04-7 CAPLUS
 CN 1H-Pyrrole-2,5-dicarboxamide, 3,4-diphenyl-N2,N5-bis(2-pyridinylmethyl)-
 (CA INDEX NAME)

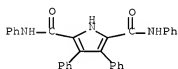


IT 365214-49-9 365214-50-2 566932-85-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of cobalt and nickel complexes of dicarboxamidopyrrole and
 dicarbothioamidopyrrole)
 RN 365214-49-9 CAPLUS
 CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-dibutyl-3,4-diphenyl- (CA INDEX NAME)



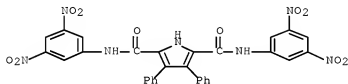
RN 365214-50-2 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5,3,4-tetraphenyl- (CA INDEX NAME)



RN 566932-85-2 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-bis(3,5-dinitrophenyl)-3,4-diphenyl-
(CA INDEX NAME)



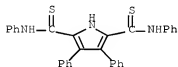
IT 1058151-99-7P 1058152-02-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation of cobalt and nickel complexes of dicarboxamidopyrrole and
dicarbothioamidopyrrole)

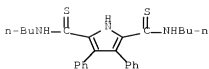
RN 1058151-99-7 CAPLUS

CN 1H-Pyrrole-2,5-dicarbothioamide, N2,N5,3,4-tetraphenyl- (CA INDEX NAME)



RN 1058152-02-5 CAPLUS

CN 1H-Pyrrole-2,5-dicarbothioamide, N2,N5-dibutyl-3,4-diphenyl- (CA INDEX
NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 43 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2008:696589 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 149:143220

TITLE: Thermodynamic and Structure Guided Design of Statin Based Inhibitors of 3-Hydroxy-3-Methylglutaryl Coenzyme A Reductase

AUTHOR(S): Sarver, Ronald W.; Bills, Elizabeth; Bolton, Gary; Bratton, Larry D.; Caspers, Nicole L.; Dunbar, James B.; Harris, Melissa S.; Hutchings, Richard H.; Kennedy, Robert M.; Larsen, Scott D.; Pavlovsky, Alexander; Pfefferkorn, Jeffrey A.; Bainbridge, Graeme
CORPORATE SOURCE: Pfizer Global Research + Development, Ann Arbor, MI, 48105, USA

SOURCE: Journal of Medicinal Chemistry (2008), 51(13), 3804-3813

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Clin. studies have demonstrated that statins, 3-hydroxy-3-methylglutaryl CoA reductase (HMGR) inhibitors, are effective at lowering mortality levels associated with cardiovascular disease; however, 2-7% of patients may experience statin-induced myalgia that limits compliance with a treatment regimen. High resolution crystal structures, thermodyn. binding parameters, and biochem. data were used to design statin inhibitors with improved HMGR affinity and therapeutic index relative to statin-induced myalgia. These studies facilitated the identification of imidazole 1 as a potent (IC₅₀ = 7.9 nM) inhibitor with excellent hepatoselectivity (>1000-fold) and good in vivo efficacy. The binding of 1 to HMGR was enthalpically driven with a ΔH of -17.7 kcal/M. Addnl., a second novel series of bicyclic pyrrole-based inhibitors was identified that induced order in a protein flap of HMGR. Similar ordering was detected in a substrate complex, but has not been reported in previous statin inhibitor complexes with HMGR.

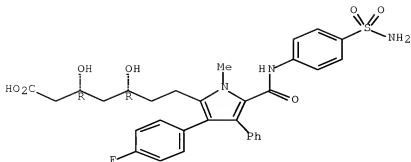
IT 1037300-11-0 1037300-16-5

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(thermodn. and structure guided design of statin based inhibitors of HMGCoA reductase)

RN 1037300-11-0 CAPLUS

CN 1H-Pyrrole-2-heptanoic acid, 5-[[[4-(aminosulfonyl)phenyl]amino]carbonyl]-3-(4-fluorophenyl)- β , δ -dihydroxy-1-methyl-4-phenyl-, (BR, δ R)- (CA INDEX NAME)

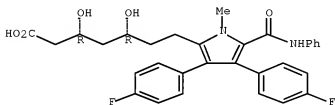
Absolute stereochemistry.



RN 1037300-16-5 CAPLUS

CN 1H-Pyrrole-2-heptanoic acid, 3,4-bis(4-fluorophenyl)-β,δ-dihydroxy-1-methyl-5-[(phenylamino)carbonyl]-, (βR,δR)- (CA INDEX NAME)

Absolute stereochemistry.



IT 1037300-12-1 1037300-13-2 1037300-14-3

1037300-15-4 1037300-17-6

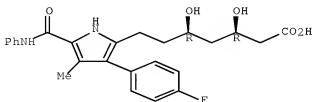
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(thermodn. and structure guided design of statin based inhibitors of HMGCoA reductase)

RN 1037300-12-1 CAPLUS

CN 1H-Pyrrole-2-heptanoic acid, 3-(4-fluorophenyl)-β,δ-dihydroxy-4-(4-fluorophenyl)-1-methyl-5-[(phenylamino)carbonyl]-, (βR,δR)- (CA INDEX NAME)

Absolute stereochemistry.

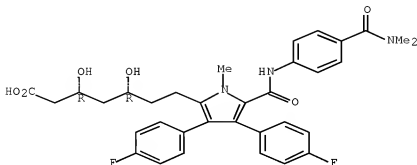


RN 1037300-13-2 CAPLUS

CN 1H-Pyrrole-2-heptanoic acid, 5-[[[4-

[(dimethylamino)carbonyl]phenyl]amino]carbonyl]-3,4-bis(4-fluorophenyl)-
 β,δ -dihydroxy-1-methyl-, ($\beta R, \delta R$)- (CA INDEX NAME)

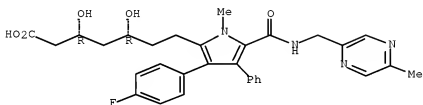
Absolute stereochemistry.



RN 1037300-14-3 CAPLUS

CN 1H-Pyrrole-2-heptanoic acid, 3-(4-fluorophenyl)- β,δ -dihydroxy-1-methyl-5-[[[4-(methoxycarbonyl)phenyl]amino]carbonyl]-4-phenyl-, ($\beta R, \delta R$)- (CA INDEX NAME)

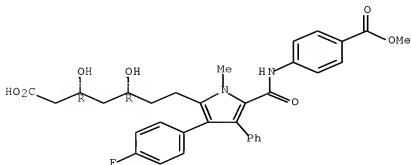
Absolute stereochemistry.



RN 1037300-15-4 CAPLUS

CN 1H-Pyrrole-2-heptanoic acid, 3-(4-fluorophenyl)- β,δ -dihydroxy-5-[[[4-(methoxycarbonyl)phenyl]amino]carbonyl]-1-methyl-4-phenyl-, ($\beta R, \delta R$)- (CA INDEX NAME)

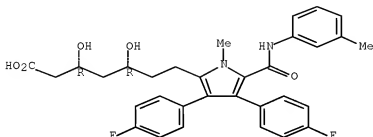
Absolute stereochemistry.



RN 1037300-17-6 CAPLUS

CN 1H-Pyrrole-2-heptanoic acid, 3,4-bis(4-fluorophenyl)- β , δ -
dihydroxy-1-methyl-5-[(3-methylphenyl)amino]carbonyl]-,
(β R, δ R)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 43 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2008:43435 CAPLUS Full-text

DOCUMENT NUMBER: 148:144656

TITLE: Preparation of pyridinonyl PDK1 inhibitors

INVENTOR(S): Lind, Kenneth Egnard; Cao, Kathy; Lin, Edward
Yin-Shiang; Nguyen, Thinh Ba; Tangonan, Bradley T.;
Erlanson, Daniel A.; Guckian, Kevin; Simmons, Robert
Lowell; Lee, Wen-Cherng; Sun, Lihong; Hansen, Stig;
Pathan, Nuzhat; Zhang, Lei
PATENT ASSIGNEE(S): Sunesis Pharmaceuticals, USA; Biogen Idec, Inc.

SOURCE: PCT Int. Appl., 31pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008005457	A2	20080110	WO 2007-US15397	20070702
WO 2008005457	A3	20080724		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			

PRIORITY APPLN. INFO.:

US 2006-806414P

P 20060630

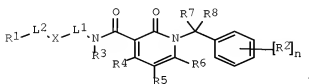
US 2007-919057P

P 20070319

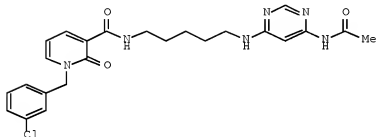
OTHER SOURCE(S):

MARPAT 148:144656

GI



I



II

AB The title compds. I [$n = 1-5$; $L_1, L_2 =$ a bond, O, NH, S, S(O), S(O) $_2$, (hetero)alkylene; X = a bond, (hetero)cycloalkylene, (hetero)arylene; $R_1 =$ (hetero)cycloalkyl, (hetero)aryl; $R_2, R_4-R_8 =$ H, halo, OH, CF $_3$, etc.; $R_3 =$ H, OH, CF $_3$, alkyl, etc.], useful as 3-phosphoinositide-dependent protein kinase-1 (PDK1) inhibitors for treating cancer, were prepared E.g., a 2-step synthesis of II, starting from tert-Bu (5-aminopentyl)carbamate and 1-(3-chlorobenzyl)-2-oxo-1,2-dihydropyridine-3-carboxylic acid, was given. Exemplified compds. I were tested for PDK1 inhibitory activity in various assays (data given). Pharmaceutical composition comprising the compound I is disclosed.

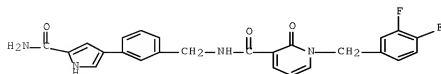
IT 1001408-63-8P 1001408-97-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyridinonyl PDK1 inhibitors for treating cancer)

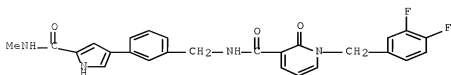
RN 1001408-83-8 CAPLUS

CN 3-Pyridinecarboxamide, N-[[3-[5-(aminocarbonyl)-1H-pyrrol-3-yl]phenyl]methyl]-1-[(3,4-difluorophenyl)methyl]-1,2-dihydro-2-oxo- (CA INDEX NAME)



RN 1001408-97-4 CAPLUS

CN 3-Pyridinecarboxamide, 1-[(3,4-difluorophenyl)methyl]-1,2-dihydro-N-[[3-[5-
[(methylanino)carbonyl]-1H-pyrrol-3-yl]phenyl)methyl]-2-oxo- (CA INDEX
NAME)



L3 ANSWER 4 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:902048 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 147:427173

TITLE: Regioselective Synthesis of Highly Aryl-Substituted
Pyrrole Carboxylates as Useful Medicinal Chemistry
Leads

AUTHOR(S): Bhatt, Ulhas; Duffy, Bryan C.; Guzzo, Peter R.; Cheng,
Leifeng; Elebring, Thomas

CORPORATE SOURCE: Albany Molecular Research, Inc., Albany, NY, USA
SOURCE: Synthetic Communications (2007), 37(16), 2793-2806

CODEN: SYNCV; ISSN: 0039-7911

PUBLISHER: Taylor & Francis, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:427173

AB The regioselective syntheses of two pharmaceutically relevant pyrrole
scaffolds are described. A synthetic route for the preparation of
differentially substituted pyrrole-3,4-dicarboxylates is presented and
exemplified. This route circumvents some of the problems and limitations
associated with previous butynedioic diester condensations and 1,3-dipolar
cycloaddn. reactions. A route to the related 4,5-diarylpyrrole-2-carboxylic
acid scaffold is also presented. Both routes allow for the regiocontrolled
preparation of highly substituted pyrrole pharmacophore cores.

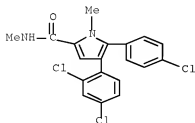
IT 952019-94-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(regioselective preparation of aryl-substituted pyrrole-3,4-dicarboxylates
and 2-pyrrolecarboxylates)

RN 952019-94-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 5-(4-chlorophenyl)-4-(2,4-dichlorophenyl)-N,1-
dimethyl- (CA INDEX NAME)

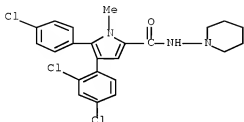


IT 875667-50-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective preparation of aryl-substituted pyrrole-3,4-dicarboxylates
and 2-pyrrolicarboxylates)

RN 875667-50-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 5-(4-chlorophenyl)-4-(2,4-dichlorophenyl)-1-
methyl-N-1-piperidinyl- (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:874967 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 147:257800

TITLE: 3,4-Dihydropyrrolo[1,2-a]pyrazin-1(2H)-ones as melanin
concentrating hormone receptor-1 antagonists and their
preparation, pharmaceutical compositions and use in
the treatment of disease

INVENTOR(S): Zhao, Guohua

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: U.S. Pat. Appl. Publ., 34pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

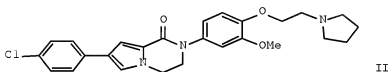
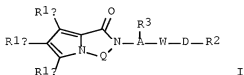
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

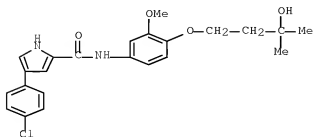
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070185097	A1	20070809	US 2007-671150	20070205
WO 2007092416	A2	20070816	WO 2007-US3099	20070206
WO 2007092416	A3	20071101		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			
EP 1987039	A2	20081105	EP 2007-763593	20070206

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
 IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
 PRIORITY APPLN. INFO.: US 2006-765530P P 20060206
 WO 2007-US3099 W 20070206
 OTHER SOURCE(S): MARPAT 147:257800
 GI



- AB The application provides compds. of formula I, including all stereoisomers, solvates, prodrugs and pharmaceutically acceptable forms thereof. Addnl., the application provides pharmaceutical compns. containing at least one compound according to formula I and optionally at least one addnl. therapeutic agent. Finally, the application provides methods for treating a patient suffering from an MCHR-1 modulated disease or disorder such as, for example, obesity, diabetes, depression or anxiety by administration of a therapeutically ED of a compound according to formula I. Compds. of formula I wherein A is monocyclic (hetero)aryl and bicyclic heteroaryl; D is a bond, alkyl, cycloalkyl and heterocyclyl; Q is (un)substituted C1-4 alkyl, (un)substituted acetyl, (un)substituted carbonyl-alkyl, CO, COCO, etc.; W is a bond, CO, O, NH and derivs., SO, SO2, SO2NH and derivs., and (un)substituted methylene; R1a, R1b, and R1c are independently H, halo, (un)substituted (hetero)aryl, (un)substituted aryloxy, (un)substituted arylthio, and (un)substituted arylalkylthio; R2 is H, OH, lower alkoxy, hydroxyalkyl, lower cycloalkoxy, OCONH2 and derivs., CN, CONH2 and derivs., etc.; R3 is H, OH, halo, alkoxy, CN, alkyl, perfluoroalkyl, cycloalkyl, etc.; and their pharmaceutically acceptable salts, stereoisomers, solvates, and prodrug esters thereof, are claimed. Example compound II•TFA was prepared by cross-coupling of Me 4-bromo-1H-pyrrole-2-carboxylate with 4-chlorophenylboronic acid; the resulting Me 4-(4-chlorophenyl)-1H-pyrrole-2-carboxylate underwent hydrolysis to give 4-(4-chlorophenyl)-1H-pyrrole-2-carboxylic acid which underwent amidation with 3-methoxy-4-(2-(pyrrolidin-1-yl)ethoxy)benzenamine to give 4-(4-chlorophenyl)-N-(3-methoxy-4-(2-(pyrrolidin-1-yl)ethoxy)phenyl)-1H-pyrrole-2-carboxamide, which underwent cyclization with 1,2-dibromoethane to give compound II•TFA. All the invention compds. were evaluated for their melanin concentrating hormone receptor-1 antagonistic activity.
- IT 1057107-73-9
 RL: PRPH (Prophetic)
 (3,4-Dihydropyrrolo[1,2-a]pyrazin-1(2H)-ones as melanin concentrating hormone receptor-1 antagonists and their preparation, pharmaceutical compositions and use in the treatment of disease)
- RN 1057107-73-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[4-(3-hydroxy-3-methylbutoxy)-3-methoxyphenyl]- (CA INDEX NAME)



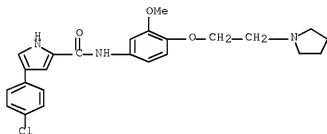
IT 945720-32-1P 945720-37-6P 945720-40-1E
 945720-43-4P 945720-44-5P 945720-45-6P
 945720-46-7P 945720-47-8P 945720-48-9P
 945720-49-0P 945720-50-3P 945720-51-4P
 945720-52-5P 945720-55-8P 945720-58-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of dihydropyrrolopyrazinones as melanin concentrating hormone receptor 1 antagonists useful alone or in combination therapy of MCHR-1 - mediated diseases)

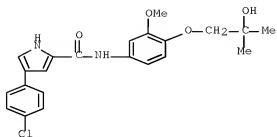
RN 945720-32-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-methoxy-4-[2-(1-pyrrolidinyl)ethoxy]phenyl]- (CA INDEX NAME)



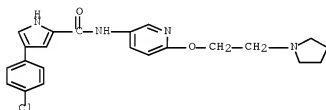
RN 945720-37-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[4-(2-hydroxy-2-methylpropoxy)-3-methoxyphenyl]- (CA INDEX NAME)



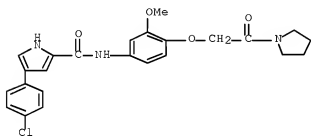
RN 945720-40-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[6-[2-(1-pyrrolidinyl)ethoxy]-3-pyridinyl]- (CA INDEX NAME)



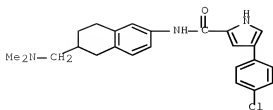
RN 945720-43-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-methoxy-4-[2-oxo-2-(1-pyrrolidinyl)ethoxy]phenyl]- (CA INDEX NAME)



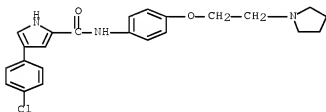
RN 945720-44-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[6-[(dimethylamino)methyl]-5,6,7,8-tetrahydro-2-naphthalenyl]- (CA INDEX NAME)



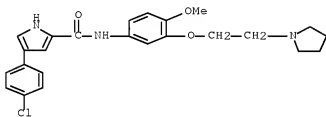
RN 945720-45-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[4-[2-(1-pyrrolidinyl)ethoxy]phenyl]- (CA INDEX NAME)



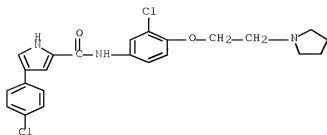
RN 945720-46-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[4-methoxy-3-[2-(1-pyrrolidinyl)ethoxy]phenyl]- (CA INDEX NAME)



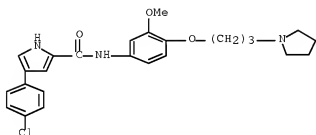
RN 945720-47-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-chloro-4-[2-(1-pyrrolidinyl)ethoxy]phenyl]- (CA INDEX NAME)



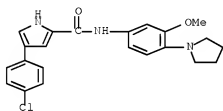
RN 945720-48-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-methoxy-4-[3-(1-pyrrolidinyl)propoxy]phenyl]- (CA INDEX NAME)



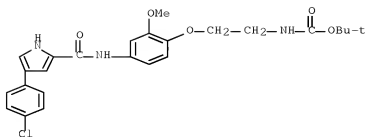
RN 945720-49-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-methoxy-4-(1-pyrrolidinyl)phenyl]- (CA INDEX NAME)



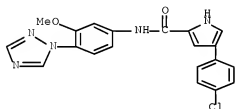
RN 945720-50-3 CAPLUS

CN Carbamic acid, N-[2-[4-[[4-(4-chlorophenyl)-1H-pyrrol-2-yl]carbonyl]amino]-2-methoxyphenoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 945720-51-4 CAPLUS

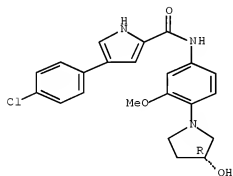
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-methoxy-4-(1H-1,2,4-triazol-1-yl)phenyl]- (CA INDEX NAME)



RN 945720-52-5 CAPLUS

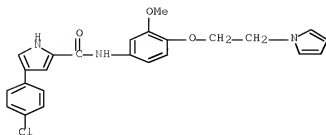
CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[4-[(3R)-3-hydroxy-1-pyrrolidinyl]-3-methoxyphenyl]- (CA INDEX NAME)

Absolute stereochemistry.

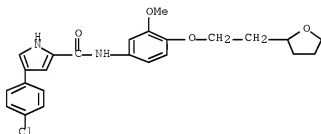


RN 945720-55-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-methoxy-4-[2-(1H-pyrrol-1-yl)ethoxy]phenyl]- (CA INDEX NAME)

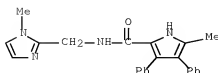


RN 945720-58-1 CAPLUS
 CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[3-methoxy-4-[2-(tetrahydro-2-furanyl)ethoxy]phenyl]- (CA INDEX NAME)



L3 ANSWER 6 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2007:450172 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 147:72319
 TITLE: Conformational control of HCl co-transporter: imidazole functionalized isophthalamide vs. 2,6-dicarboxamidopyridine
 AUTHOR(S): Gale, Philip A.; Garric, Joachim; Light, Mark E.; McNally, Beth A.; Smith, Bradley D.
 CORPORATE SOURCE: School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
 SOURCE: Chemical Communications (Cambridge, United Kingdom) (2007), (17), 1736-1738
 CODEN: CHCOFS; ISSN: 1359-7345
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 147:72319
 AB Replacement of the central isophthalamide core in a synthetic HCl receptor, with a 2,6-dicarboxamidopyridine, leads to a more preorganized mol. structure that exhibits higher chloride affinity and membrane transport flux.
 IT 864943-19-1
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
 (inclusion reaction; conformational control of HCl co-transporter by imidazole functionalized isophthalamide vs. 2,6-dicarboxamidopyridine)
 RN 864943-19-1 CAPLUS
 CN 1H-Pyrrole-2-carboxamide, 5-methyl-N-[(1-methyl-1H-imidazol-2-yl)methyl]-

3,4-diphenyl- (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1356739 CAPLUS Full-text
DOCUMENT NUMBER: 146:121812
TITLE: 4,5-Diarylpyrrole derivatives, their preparation, and
their therapeutic application as cannabinoid CB1
receptor antagonists
INVENTOR(S): Barth, Francis; Congy, Christian; Hortala, Laurent;
Rinaldi-Carmona, Murielle
PATENT ASSIGNEE(S): Sanofi Aventis, Fr.
SOURCE: Fr. Demande, 28pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2887548	A1	20061229	FR 2005-6609	20050627
FR 2887548	B1	20070921		
AU 2006263781	A1	20070104	AU 2006-263781	20060622
CA 2610805	A1	20070104	CA 2006-2610805	20060622
WO 2007000505	A2	20070104	WO 2006-FR1416	20060622
WO 2007000505	A3	20071115		
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RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			
EP 1899298	A2	20080319	EP 2006-764809	20060622
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US 20080176924	A1	20080724	US 2007-952224	20071207
IN 2007KN04798	A	20080215	IN 2007-KN4798	20071210
MX 200716383	A	20080307	MX 2007-16383	20071218
KR 2008019641	A	20080304	KR 2007-730262	20071226
CN 101208300	A	20080625	CN 2006-80023067	20071222

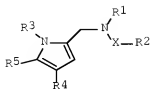
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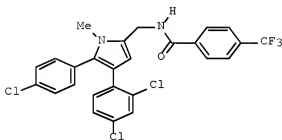
NO 2008-458
FR 2005-6609
WO 2006-FR1416

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A 20050627
W 20060622

OTHER SOURCE(S): MARPAT 146:121812
GI



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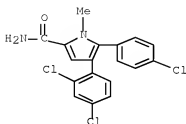


II

- AB The invention provides compds. I [X = CO, SO₂, or CON(R₆); R₁ = H or C1-4 alkyl; R₂ = C1-7 alkyl, nonarom. C3-12 carbocyclyl optionally substituted by C1-4 alkyl and optionally attached via CH₂, (un)substituted Ph, (un)substituted benzyl, benzhydryl, benzhydrylmethyl, 1,2,3,4-tetrahydronaphthalen-2-yl optionally substituted by C1-4 alkyl, heterocycles (pyrrolyl, imidazolyl, pyridyl, pyrazolyl, furyl, or thienyl) optionally substituted by alkyl and/or halo, indol-2-yl, N-methylindol-2-yl; R₃ = C1-5 alkyl or C3-7 cycloalkyl; R₄, R₅ = (un)substituted Ph; R₆ = H or C1-4 alkyl; including bases, acid addition salts, hydrates, and/or solvates]. Also provided are a process for preparing I, and therapeutic applications of I. Claimed uses include the treatment or prevention of appetite disorders, metabolic disorders, gastrointestinal diseases, inflammatory phenomena, immune system disorders, psychotic disorders, alc. dependence, and nicotine dependence. Eighteen compds. I are described in detail, 13 of which were prepared by combinatorial methods. For instance, the ester Me 5-(4-chlorophenyl)-4-(2,4-dichlorophenyl)-1H-pyrrole-2-carboxylate (prepared in 5 steps) underwent a sequence of 4 steps (hydrolysis, amidation, reduction of the carboxamide to a methylamine, and amidation of the amine with the corresponding acid chloride) to give invention compound II. Compds. I have very good in vitro affinity for cannabinoid CB₁ receptors, with IC₅₀ ≤ 5·10⁻⁷M. The antagonist nature of compds. I was demonstrated by adenylyl-cyclase inhibition models, and toxicity was compatible with therapeutic use (no data).
- IT 918294-12-9P, 5-(4-Chlorophenyl)-4-(2,4-dichlorophenyl)-1-methyl-1H-pyrrole-2-carboxamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of diarylpyrrole derivs. as cannabinoid CB₁ receptor antagonists)

RN 918294-12-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 5-(4-chlorophenyl)-4-(2,4-dichlorophenyl)-1-methyl- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:699903 CAPLUS Full-text

DOCUMENT NUMBER: 145:145/09

TITLE: Preparation of heterocyclic carboxamide compounds as steroid nuclear receptors ligands

INVENTOR(S): Flatt, Brenton; Gu, Xiao-Hui; Martin, Richard; Mohan, Raju; Murphy, Brett; Nyman, Michael C.; Stevens, William C., Jr.; Wang, Tie-Lin

PATENT ASSIGNEE(S): Exelixis, Inc., USA

SOURCE: PCT Int. Appl., 196 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

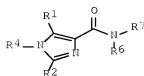
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006076202	A1	20060720	WO 2006-US319	20060106
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
AU 2006205220	A1	20060720	AU 2006-205220	20060106
CA 2593156	A1	20060720	CA 2006-2593156	20060106
EP 1844020	A1	20071017	EP 2006-717506	20060106
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU			
JP 2008526869	T	20080724	JP 2007-550462	20060106
PRIORITY APPLN. INFO.:			US 2005-642839P	P 20050110

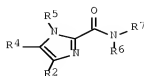
OTHER SOURCE(S):

MARPAT 145:145709

GI



I



II

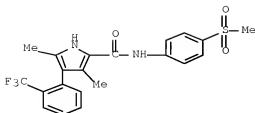
AB Imidazole-4-carboxamides (I) and imidazole-2-carboxamide (II) [R1, R2 = H, cyano, halo, each (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl, heteroaryl, or heteroaralkyl; R5 = H, each alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl, heteroaryl, or heteroaralkyl; R4 = each (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, aralkyl, heteroaryl, or heteroaralkyl; R6 = H; R7 = each (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, aralkyl, heteroaryl or heteroaralkyl] as single isomers, mixture of isomers, or as racemic mixts. of isomers or as solvates or polymorphs or as prodrugs or metabolites or as pharmaceutically acceptable salts thereof are prepared. These compds. are useful in modulating the activity of steroid nuclear receptors and thereby for the treatment of a disease, or disorder mediated by, or otherwise affected by one or more steroid nuclear receptors (in particular mineralocorticoid receptor), or in which steroid nuclear receptor activity is implicated. The above disease or disorder is related to cancer, infertility, one or more metabolic syndromes, bone or cartilage dysfunction, immune dysfunction, cognitive dysfunction, high blood pressure, heart disease, renal disease, fibrosis, epidermal dysfunction, or muscle wasting. Thus, to a stirred mixture of 1,4-dimethyl-5-(2-phenoxyphenyl)-1H-imidazole-2-carboxylic acid Et ester (202 mg, 0.60 mmol) and 4-methanesulfonylaniline (136 mg, 0.80 mmol) in toluene (5 mL, anhydrous) was added dropwise Me3Al (2.0 M in toluene, 0.4 mL, 0.8 mmol) under N at ambient temperature and the resulting mixture was stirred at 100° in a sealed vial for 10 h to give, after silica gel chromatog., 1,4-dimethyl-5-(2-phenoxyphenyl)-1H-imidazole-2-carboxylic acid (4-methanesulfonylphenyl)amide (III). III showed antagonist activity against mineralocorticoid receptor with IC50 of <0.5 μ M which was ten-fold greater than the antagonist activity against androgen receptor (AR), estrogen receptor α (ER α), glucocorticoid receptor (GR), and progesterone receptor (PR).

IT 880779-28-2P, 3,5-Dimethyl-4-(2-trifluoromethylphenyl)-1H-pyrrole-2-carboxylic acid N-(4-methylsulfonylphenyl)amide
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of imidazolecarboxamides as modulators of steroid nuclear receptors)

RN 880779-28-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 3,5-dimethyl-N-[4-(methylsulfonyl)phenyl]-4-[2-(trifluoromethyl)phenyl]- (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 9 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:640343 CAPLUS Full-text

DOCUMENT NUMBER: 145:188387

TITLE: Pyrrolylamidourea based anion receptors

AUTHOR(S): Evans, Louise S.; Gale, Philip A.; Light, Mark E.; Quesada, Roberto

CORPORATE SOURCE: School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK

SOURCE: New Journal of Chemistry (2006), 30(7), 1019-1025

CODEN: NJCHE5; ISSN: 1144-0546

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:188387

AB The anion binding behavior of a number of pyrrolylamidourea and thiourea compds. have been studied in DMSO solution Mono-amidothioureapyrrole compds. were found to be deprotonated by basic anions such as fluoride, acetate, benzoate or dihydrogenphosphate with the structure of the deprotonated species elucidated by X-ray crystallog. 2,5-Bis(amidourea)pyrroles were synthesized and found to be effective anion receptors for a range of putative anionic guests.

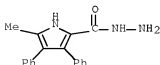
IT 884529-86-6P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(crystallog.; addition to aryl isocyanate; pyrrolylamidourea based anion receptors)

RN 884529-86-6 CAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-, hydrazide (CA INDEX NAME)



IT 884529-86-6P

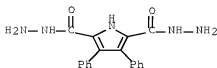
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(crystallog.; addition to aryl isocyanate; pyrrolylamidourea based anion

receptors)

RN 902141-41-7 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxylic acid, 3,4-diphenyl-, 2,5-dihydrazide (CA INDEX NAME)



IT 902141-43-9

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(crystallog.; pyrrolylamidourea based anion receptors)

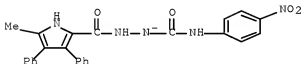
RN 902141-43-9 CAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, 5-methyl-3,4-diphenyl-1H-pyrrole-2-carboxylic acid hydrazide (1:1) (CA INDEX NAME)

CM 1

CRN 902141-42-8

CMF C25 H20 N5 O4



CM 2

CRN 10549-76-5

CMF C16 H36 N



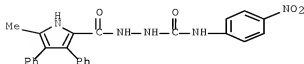
IT 884529-83-3P 902141-33-7P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(crystallog.; pyrrolylamidourea based anion receptors)

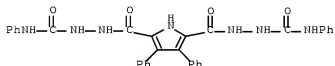
RN 884529-83-3 CAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-,
2-[[{(4-nitrophenyl)amino}carbonyl]hydrazide] (CA INDEX NAME)



RN 902141-33-7 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxylic acid, 3,4-diphenyl-,
2,5-bis[2-[(phenylamino)carbonyl]hydrazide] (CA INDEX NAME)

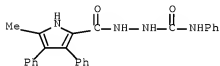


IT 884529-82-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(no association with anions; pyrrolylamidourea based anion receptors)

RN 884529-82-2 CAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-,
2-[(phenylamino)carbonyl]hydrazide (CA INDEX NAME)

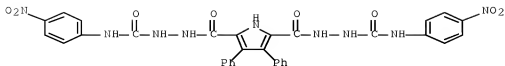


IT 902141-35-9P 902141-37-1P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP
(Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC
(Process)
(pyrrolylamidourea based anion receptors)

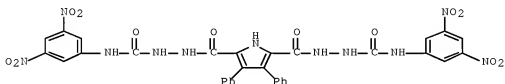
RN 902141-35-9 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxylic acid, 3,4-diphenyl-,
2,5-bis[2-[[{(4-nitrophenyl)amino}carbonyl]hydrazide] (CA INDEX NAME)



RN 902141-37-1 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxylic acid, 3,4-diphenyl-,
2,5-bis[2-[(3,5-dinitrophenyl)amino]carbonyl]hydrazide] (CA INDEX NAME)

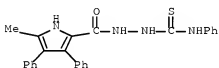


IT 884529-84-4P 884529-85-5P

RL: PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process) (pyrrolylamidourea based anion receptors)

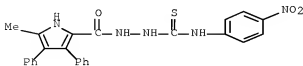
RN 884529-84-4 CAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-,
2-[(phenylamino)thioxomethyl]hydrazide (CA INDEX NAME)



RN 884529-85-5 CAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-,
2-[[4-nitrophenyl)amino]thioxomethyl]hydrazide (CA INDEX NAME)



REFERENCE COUNT:

29

THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:332235 CAPLUS Full-text

DOCUMENT NUMBER: 144:350539

TITLE: Preparation of pyrrolecarboxamide derivatives as mineralocorticoid receptor antagonists for use against cancer and other disorders

INVENTOR(S): Canne Bannen, Lynne; Chen, Jeff; Dalrymple, Lisa
Esther; Flatt, Brenton T.; Forsyth, Timothy Patrick;
Gu, Xiao-Hu; Mac, Morrison B.; Mann, Larry W.; Mann,
Grace; Martin, Richard; Mohan, Raju; Murphy, Brett;
Nyman, Michael Charles; Stevens, William C., Jr.;
Wang, Tie-Lin; Wong, Yong; Wu, Jason H.

PATENT ASSIGNEE(S): Exelixis, Inc., USA

SOURCE: PCT Int. Appl., 477 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

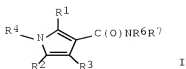
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

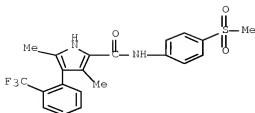
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006012642	A2	20060202	WO 2005-US26916	20050730
WO 2006012642	A3	20060727		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
AU 2005266890	A1	20060202	AU 2005-266890	20050730
CA 2573426	A1	20060202	CA 2005-2573426	20050730
EP 1773768	A2	20070418	EP 2005-803281	20050730
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU			
CN 101006052	A	20070725	CN 2005-80026842	20050730
BR 2005013677	A	20071127	BR 2005-13677	20050730
JP 2008508308	T	20080321	JP 2007-523832	20050730
IN 2007DN00605	A	20070817	IN 2007-DN605	20070123
NO 2007000910	A	20070426	NO 2007-910	20070216
KR 2007045283	A	20070502	KR 2007-704302	20070223
US 20080234270	A1	20080925	US 2007-572962	20071203
PRIORITY APPLN. INFO.:			US 2004-592439P	P 20040730
			US 2004-592469P	P 20040730
			WO 2005-US26916	W 20050730

OTHER SOURCE(S): MARPAT 144:350539

GI



- AB Pyrrolecaboxamide derivs. (shown as I; other Markush structures for pyrrolecaboxamides are defined in the claims; variables defined below; e.g. 1-[4-fluoro-2-(trifluoromethyl)phenyl]-2,5-dimethyl-1H-pyrrole-3- carboxylic acid N-[4-(sulfamoyl)phenyl]amide (II)), compns. and methods for modulating the activity of receptors are provided. In particular compds. and compns. are provided for modulating the activity of receptors and for the treatment, prevention, or amelioration of ≥ 1 symptoms of disease or disorder directly or indirectly related to the activity of the receptors. Semiquant. IC50 values for antagonist activity of 23 examples of I are tabulated and compared to the activity of the Spironolactone control. For I: R1 and R2 = H, halo, cyano, or (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl, heteroaryl, heteroaralkyl, heterocyclyl, or heterocyclylalkyl, or -OR9, -SR9, -N(R9)2, -C(O)OR9 or -C(O)N(R9)2; R3 = H, halo, cyano, (un)substituted alkyl, (un)substituted alkenyl or (un)substituted alkynyl; R4 is H, -C(O)R9, -S(O)2R9, or (un)substituted alkyl, alkenyl or alkynyl, or R4 is (un)substituted cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, aralkyl, heteroaryl or heteroaralkyl; R6 is H or (un)substituted alkyl; R7 is (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, aralkyl, heteroaryl or heteroaralkyl; addnl. details are given in the claims. Although the methods of preparation are not claimed, preps. and/or characterization data for many examples of I are included. For example, II was prepared in 5 steps (50, 37, 62, 64, and 66 % yields, resp.) starting with preparation of 1-[4-fluoro-2-(trifluoromethyl)phenyl]-2,5-dimethyl-1H-pyrrole from 4-fluoro-2-(trifluoromethyl)aniline and 2,5-hexanedione, followed by preparation of the following intermediates: 1-(4-fluoro-2-trifluoromethylphenyl)-2,5-dimethyl-1H-pyrrole-3- carboxaldehyde, 1-[4-fluoro-2-(trifluoromethyl)phenyl]-2,5-dimethyl-1H- pyrrole-3-carboxylic acid, and 1-[4-fluoro-2-(trifluoromethyl)phenyl]-2,5- dimethyl-1H-pyrrole-3-carbonyl chloride and finally amide formation with sulfanilamide.
- IT 880779-28-2P, 3,5-Dimethyl-4-(2-trifluoromethylphenyl)-1H-pyrrole-2-carboxylic acid N-(4-methylsulfonylphenyl)amide
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug candidate; preparation of pyrrolecaboxamide derivs. as mineralocorticoid receptor antagonists for use against cancer and other disorders)
- RN 880779-28-2 CAPLUS
- CN 1H-Pyrrole-2-carboxamide, 3,5-dimethyl-N-[4-(methylsulfonyl)phenyl]-4-[2-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L3 ANSWER 11 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:239131 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 144:467975

TITLE: Synthesis and Anion Binding Properties of N,N'-Bispyrrol-2-yl-2,5-diamidopyrrole

AUTHOR(S): Sessler, Jonathan L.; Pantos, G. Dan; Gale, Philip A.; Light, Mark E.

CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute for Cellular and Molecular Biology, University of Texas at Austin, Austin, TX, 78712-0165, USA

SOURCE: Organic Letters (2006), 8(8), 1593-1596

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:467975

AB A bispyrrol-2-yl-2,5-diamidopyrrole has been synthesized and shown to have a significantly higher affinity for oxo-anions than previous generation 2,5-diamidopyrroles.

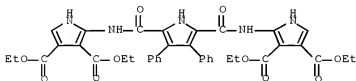
IT 886589-23-7P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and anion binding of a 3,4-diphenyl-2,5-bis(2-pyrrolylcarbamoyl)pyrrole)

RN 886589-23-7 CAPLUS

CN 1H-Pyrrole-3,4-dicarboxylic acid, 2,2'-[(3,4-diphenyl-1H-pyrrole-2,5-diyl)bis(carbonylimino)]bis-, tetraethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

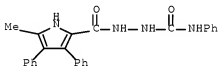
L3 ANSWER 12 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:160694 CAPLUS [Full-text](#)

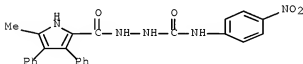
DOCUMENT NUMBER: 144:424677

TITLE: Anion binding vs. deprotonation in colorimetric

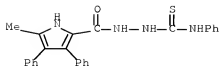
AUTHOR(S): pyrrolylamidothiourea based anion sensors
 Evans, Louise S.; Gale, Philip A.; Light, Mark E.;
 Quesada, Roberto
 CORPORATE SOURCE: School of Chemistry, University of Southampton,
 Southampton, SO17 1BJ, UK
 SOURCE: Chemical Communications (Cambridge, United Kingdom)
 (2006), (9), 965-967
 CODEN: CHCOFS; ISSN: 1359-7345
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 144:424677
 AB A pyrrolylamidothiourea deprotonates in the presence of one equivalent of not
 only fluoride, but also acetate, benzoate or dihydrogen phosphate in DMSO
 solution with structural studies using synchrotron radiation confirming
 thiourea deprotonation in the solid state.
 IT 884529-82-2P 884529-83-3P 884529-84-4P
 884529-85-5P
 RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic
 preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
 (anion binding vs. deprotonation in colorimetric pyrrolylamidothiourea
 based anion sensors)
 RN 884529-82-2 CAPLUS
 CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-,
 2-[(phenylamino)carbonyl]hydrazide (CA INDEX NAME)



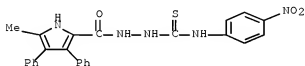
RN 884529-83-3 CAPLUS
 CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-,
 2-[[4-(4-nitrophenyl)amino]carbonyl]hydrazide (CA INDEX NAME)



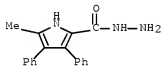
RN 884529-84-4 CAPLUS
 CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-,
 2-[(phenylamino)thioxomethyl]hydrazide (CA INDEX NAME)



RN 884529-85-5 CAPLUS
 CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-,
 2-[[[(4-nitrophenyl)amino]thioxomethyl]hydrazide (CA INDEX NAME)



IT 884529-86-6P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (preparation and use in preparation of pyrrolylamidothiourea)
 RN 884529-86-6 CAPLUS
 CN 1H-Pyrrole-2-carboxylic acid, 5-methyl-3,4-diphenyl-, hydrazide (CA INDEX
 NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 13 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2006:128973 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 144:440844
 TITLE: Anion binding properties of diamide derivatives of
 pyrrole-2, 5-diacetic acid in different solvents
 AUTHOR(S): Li, Rong-qing; Gao, Zhi-hong
 CORPORATE SOURCE: Department of Chemistry, Jiangsu Province Key
 Laboratory for Chemistry of Low-Dimensional Materials,
 Huaiyin Teachers College, Huaian, 223300, Peop. Rep.
 China
 SOURCE: Henan Shifan Daxue Xuebao, Ziran Kexueban (2005),
 33(4), 80-82, 125
 CODEN: HESKER; ISSN: 1000-2367
 PUBLISHER: Henan Shifan Daxue Xuebao Bianjibu
 DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB The anion binding properties of diamide derivs. of pyrrole-2,5-diacetic acid in different solvents were investigated, using 1H NMR titration techniques. These derivs. are shown to be effective receptors for oxo-anions in acetonitrile-d3 solution, with comparable binding affinities to those found for simple pyrrole-2,5-dicarboxamides, despite possessing a more flexible hydrogen bonding array. However, they display reduced affinities for all the anions studied in a more competitive solvent, DMSO-d6, as compared to the association consts. measured in acetonitrile-d3.

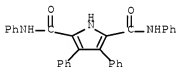
IT 365214-50-2

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(anion binding properties of diamide derivs. of pyrrole-2, 5-diacetic acid in different solvents studied by using 1H NMR titration techniques)

RN 365214-50-2 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5,3,4-tetraphenyl- (CA INDEX NAME)



L3 ANSWER 14 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:126304 CAPLUS Full-text

DOCUMENT NUMBER: 144:212649

TITLE: Preparation of 4,5-diphenylpyrrole-2-carboxamide derivatives as antagonists of CB1 cannabinoid receptors and their therapeutic application

INVENTOR(S): Barth, Francis; Congy, Christian; Hortala, Laurent; Rinaldi Carmona, Murielle

PATENT ASSIGNEE(S): Sanofi-Synthelabo, Fr.

SOURCE: Fr. Demande, 26 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2874012	A1	20060210	FR 2004-8773	20040809
FR 2874012	B1	20080822		
AU 2005279086	A1	20060309	AU 2005-279086	20050802
CA 2576717	A1	20060309	CA 2005-2576717	20050802
WO 2006024777	A1	20060309	WO 2005-FR2015	20050802

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,

	CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM		
EP 1781636	A1	20070509	EP 2005-796087 20050802
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU		
CN 101014588	A	20070808	CN 2005-80030251 20050802
JP 2008509202	T	20080327	JP 2007-525320 20050802
BR 2005014235	A	20080603	BR 2005-14235 20050802
US 20070149596	A1	20070628	US 2007-625616 20070122
US 7381727	B2	20080603	
IN 2007KN00337	A	20070706	IN 2007-KN337 20070131
MX 200701383	A	20070419	MX 2007-1383 20070202
NO 2007001209	A	20070305	NO 2007-1209 20070305
KR 2007054649	A	20070529	KR 2007-705467 20070308
US 20080194581	A1	20080814	US 2008-102412 20080414
PRIORITY APPLN. INFO.:			FR 2004-8773 A 20040809 WO 2005-FR2015 W 20050802 US 2007-625616 A1 20070122

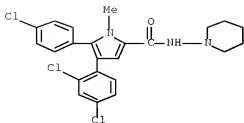
OTHER SOURCE(S): MARPAT 144:212649
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1 = H, alkyl; R2 = alkyl, 1,2,3,4-tetrahydronaphthalen-1-yl, 1,2,3,4-tetrahydronaphthalen-2-yl, (un)substituted heterocyclyl, phenylalkylene, etc.; or NR1R2 = (un)substituted piperazin-1-yl, 1,4-diazepan-1-yl, piperidin-1-yl, pyrrolidin-1-yl; R3-R8 = independently H, halo, alkyl, alkoxy, CF₃, etc.; R9 = alkyl; and their free bases, and their acid addition salts, hydrates and solvates] were prepared as antagonists of CB1 cannabinoid receptors and for treatment of the diseases it implies. For instance, II (m.p. = 165°) was prepared in 7 steps via cyclization of alkyne III (preparation given) in the presence of I₂/K₂CO₃, Pd-coupling with (2,4-dichlorophenyl)boronic acid, Ts-deprotection, alkylation of the pyrrole IV with MeI in the presence of K₂CO₃/ester hydrolysis (ester not isolated) and amidation of the acid with N-aminopiperidine. I exhibited an excellent affinity in vitro (IC₅₀ ≤ 5•10⁻⁷ M) for the CB1 cannabinoid receptors. Thus, I are useful for treating psychosis, appetite and gastrointestinal disorders, smoking and alc. cessation, etc.

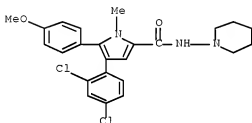
IT 875667-50-8F, 5-(4-Chlorophenyl)-4-(2,4-dichlorophenyl)-1-methyl-N-(piperidin-1-yl)-1H-pyrrole-2-carboxamide 875667-52-0F
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug candidate; preparation of pyrrole carboxamide derivs. as antagonists of CB1 cannabinoid receptors)

RN 875667-50-8 CAPLUS
 CN 1H-Pyrrole-2-carboxamide, 5-(4-chlorophenyl)-4-(2,4-dichlorophenyl)-1-methyl-N-1-piperidinyl- (CA INDEX NAME)



RN 875667-52-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2,4-dichlorophenyl)-5-(4-methoxyphenyl)-1-methyl-N-1-piperidinyl- (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 15 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:104702 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 144:462886

TITLE: Co-transport of H⁺/Cl⁻ by a synthetic prodigiosin mimic. [Erratum to document cited in CA143:300973]

AUTHOR(S): Gale, Philip A.; Light, Mark E.; McNally, Beth; Navakhun, Korakot; Sliwinski, Kate E.; Smith, Bradley D.

CORPORATE SOURCE: School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2006), (2), 226

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

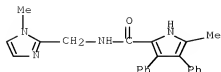
AB The structural formula for compound 2 on page 3773 was incorrect. The correct version of compound 2 is given.

IT 864943-19-1P

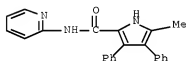
RL: BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (cotransport of H⁺/Cl⁻ by synthetic prodigiosin mimic (Erratum))

RN 864943-19-1 CAPLUS

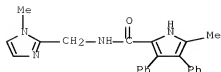
CN 1H-Pyrrole-2-carboxamide, 5-methyl-N-[(1-methyl-1H-imidazol-2-yl)methyl]-3,4-diphenyl- (CA INDEX NAME)



IT 864943-20-4P
 RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (cotransport of H⁺/Cl⁻ by synthetic prodigiosin mimic (Erratum))
 RN 864943-20-4 CAPLUS
 CN 1H-Pyrrole-2-carboxamide, 5-methyl-3,4-diphenyl-N-2-pyridinyl- (CA INDEX NAME)



L3 ANSWER 16 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:645311 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 143:300973
 TITLE: Co-transport of H⁺/Cl⁻ by a synthetic prodigiosin mimic
 AUTHOR(S): Gale, Philip A.; Light, Mark E.; McNally, Beth; Navakhun, Korakot; Sliwinski, Kate E.; Smith, Bradley D.
 CORPORATE SOURCE: School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
 SOURCE: Chemical Communications (Cambridge, United Kingdom) (2005), (30), 3773-3775
 CODEN: CHCOFS; ISSN: 1359-7345
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 143:300973
 AB An amidopyrrole with appended imidazole group can bind and co-transport H⁺/Cl⁻ across vesicle membranes much more effectively than an analog with an appended pyridyl group.
 IT 864943-19-1P
 RL: BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (cotransport of H⁺/Cl⁻ by synthetic prodigiosin mimic)
 RN 864943-19-1 CAPLUS
 CN 1H-Pyrrole-2-carboxamide, 5-methyl-N-[(1-methyl-1H-imidazol-2-yl)methyl]-3,4-diphenyl- (CA INDEX NAME)

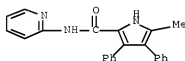


IT 864943-20-4P

RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cotransport of H⁺/Cl⁻ by synthetic prodigiosin mimic)

RN 864943-20-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 5-methyl-3,4-diphenyl-N-2-pyridinyl- (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 17 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:469894 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:7592

TITLE: Preparation of arylpyrrolecarboxamides as Raf kinase inhibitors for treatment of tumors.

INVENTOR(S): Finsinger, Dirk; Buchstaller, Hans-Peter; Burgdorf, Lars; Wiesner, Matthias; Amendt, Christiane; Grell, Matthias; Sirrenberg, Christian; Zenke, Frank

PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany

SOURCE: Ger. Offen., 32 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10354060	A1	20050602	DE 2003-10354060	20031119
AU 2004291255	A1	20050602	AU 2004-291255	20041026
CA 2546334	A1	20050602	CA 2004-2546334	20041026
WO 2005049603	A1	20050602	WO 2004-EP12076	20041026
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,				

EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
SN, TD, TG

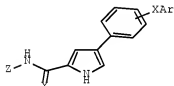
EP 1685125	A1	20060802	EP 2004-790859	20041026
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK			
CN 1882571	A	20061220	CN 2004-80034345	20041026
BR 2004016690	A	20070130	BR 2004-16690	20041026
JP 2007511553	T	20070510	JP 2006-540216	20041026
IN 2006KN00936	A	20070420	IN 2006-KN936	20060417
MX 2006PA05478	A	20060811	MX 2006-PA5478	20060515
KR 2006118492	A	20061123	KR 2006-709552	20060517
US 20070149594	A1	20070628	US 2006-579825	20060517

PRIORITY APPLN. INFO.:

DE 2003-10354060	A	20031119
WO 2004-EP12076	W	20041026

OTHER SOURCE(S): MARPAT 143:7592

GI



AB Title compds. [I; Ar = (substituted) Ph, naphthyl, biphenyl, heterocyclyl; X = O, S, (CH₂)_n, CO, (CH₂)_nO, (CH₂)_nNH, etc.; n = 1-3; Y = O, S, CHNO₂, C(CN)₂, NR₄; R₄ = H, cyano, OH, etc.; Z = Ar, ArXAr, CH₂Ar, CH₂ArXAr; Ar = (substituted) Ph], were prepared as Raf kinase inhibitors (no data). Thus, 4-(PhCH₂O)C₆H₄CH₂CO₂H, DMF, and POC13 were heated together at 70° for 4 h followed by cooling and addition of ice water and aqueous NaClO₄ to give 98% [2-(4-benzyloxyphenyl)-3-dimethylaminoallylidene]dimethylammonium perchlorate. This was refluxed 24 h with glycine Et ester hydrochloride in EtOH containing 20% NaOEt to give 91% Et 4-(4-benzyloxyphenyl)-1H-pyrrole-2-carboxylate. Hydrogenolysis of the latter in EtOAc over Pd/C gave 91% Et 4-(4-hydroxyphenyl)-1H-pyrrole-2-carboxylate. This was heated with 4-chloropyridine-2-carboxylic acid N-methylamide at 160° for 48 h to give 40% Et 4-[4-(2-methylcarbamoylpyridin-4-yloxy)phenyl]-1H-pyrrole-2-carboxylate. Saponification with 2N NaOH in EtOH at 60° for 16 h followed by acidification with HCl gave 85% free acid, which was stirred 48 h in DMF with 5-amino-2-chlorobenzotrifluoride, N-(3-dimethylaminopropyl)-N'-ethylcarbodiimide hydrochloride, and 1-hydroxybenzotriazole hydrate to give 17% 4-[4-[5-(4-chloro-3-trifluoromethylphenylcarbamoyl)-1H-pyrrol-3-yl]phenoxy]pyridine-2-carboxylic acid N-methylamide.

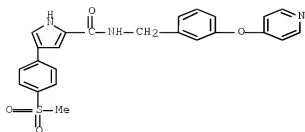
IT 1073641-53-8 1073641-54-9 1073641-55-0
1073641-56-1 1073641-58-3 1073641-59-4
1073641-60-7 1073641-61-8 1073641-62-9
1073641-63-0 1073641-64-1

RL: PRPH (Prophetic)

(Preparation of arylpyrrolecarboxamides as Raf kinase inhibitors for treatment of tumors.)

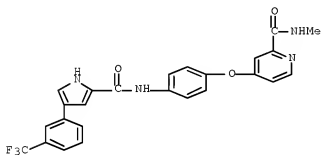
RN 1073641-53-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[4-(methylsulfonyl)phenyl]-N-[3-(4-pyridinyloxy)phenyl]methyl]- (CA INDEX NAME)



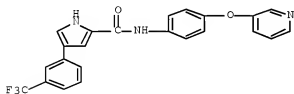
RN 1073641-54-9 CAPLUS

CN 2-Pyridinecarboxamide, N-methyl-4-[[4-[3-(trifluoromethyl)phenyl]-1H-pyrrol-2-yl]carbonylamino]phenoxy]- (CA INDEX NAME)



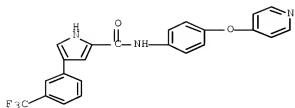
RN 1073641-55-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[4-(3-pyridinyloxy)phenyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



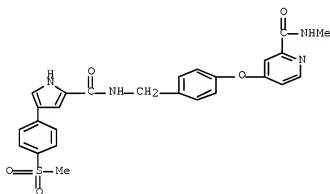
RN 1073641-56-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[4-(4-pyridinyloxy)phenyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



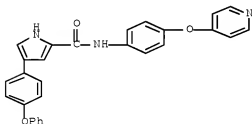
RN 1073641-58-3 CAPLUS

CN 2-Pyridinecarboxamide, N-methyl-4-[[[4-(4-(methylsulfonyl)phenyl)-1H-pyrrol-2-yl]carbonyl]amino]methyl]phenoxy]- (CA INDEX NAME)



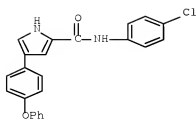
RN 1073641-59-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-phenoxyphenyl)-N-[4-(4-pyridinyloxy)phenyl]- (CA INDEX NAME)



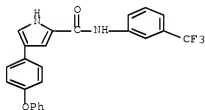
RN 1073641-60-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-(4-(4-chlorophenyl)-4-(4-phenoxyphenyl))- (CA INDEX NAME)



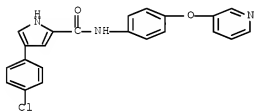
RN 1073641-61-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-phenoxyphenyl)-N-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



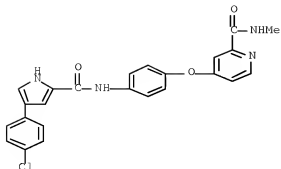
RN 1073641-62-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-[4-(3-pyridinyloxy)phenyl]- (CA INDEX NAME)



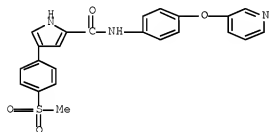
RN 1073641-63-0 CAPLUS

CN 2-Pyridinecarboxamide, 4-[4-[[[4-(4-chlorophenyl)-1H-pyrrol-2-yl]carbonyl]aminophenoxy]-N-methyl- (CA INDEX NAME)



RN 1073641-64-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[4-(methylsulfonyl)phenyl]-N-[4-(3-pyridinyloxy)phenyl]- (CA INDEX NAME)

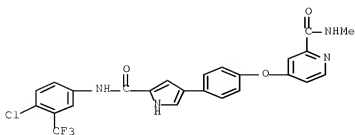


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852455-22-2P 852455-23-3P 852455-24-4P
852455-25-5P 852455-26-6P 852455-27-7P
852455-28-8P 852455-29-9P 852455-30-2P
852455-31-3P 852455-32-4P 852455-33-5P
852455-34-6P 852455-35-7P 852455-36-8P
852455-37-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of arylpyrrolicarboxamides as Raf kinase inhibitors for treatment of tumors)

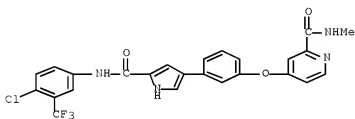
RN 852455-19-7 CAPLUS

CN 2-Pyridinecarboxamide, 4-[4-[5-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



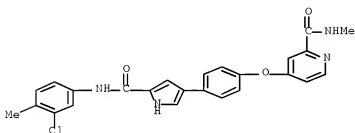
RN 852455-20-0 CAPLUS

CN 2-Pyridinecarboxamide, 4-[3-[5-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



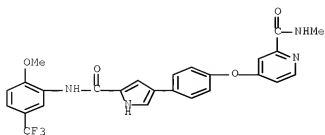
RN 852455-21-1 CAPLUS

CN 2-Pyridinecarboxamide, 4-[4-[5-[[[3-chloro-4-methylphenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



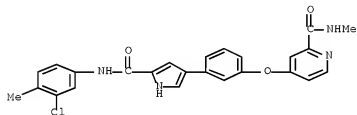
RN 852455-22-2 CAPLUS

CN 2-Pyridinecarboxamide, 4-[4-[5-[[[2-methoxy-5-(trifluoromethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



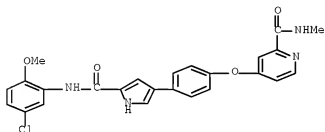
RN 852455-23-3 CAPLUS

CN 2-Pyridinecarboxamide, 4-[3-[5-[(3-chloro-4-methylphenyl)amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



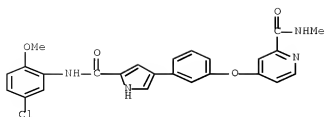
RN 852455-24-4 CAPLUS

CN 2-Pyridinecarboxamide, 4-[4-[5-[(5-chloro-2-methoxyphenyl)amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



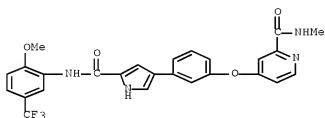
RN 852455-25-5 CAPLUS

CN 2-Pyridinecarboxamide, 4-[3-[5-[(5-chloro-2-methoxyphenyl)amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



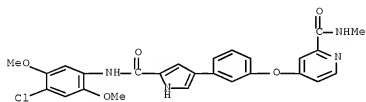
RN 852455-26-6 CAPLUS

CN 2-Pyridinecarboxamide, 4-[3-[5-[[2-methoxy-5-(trifluoromethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



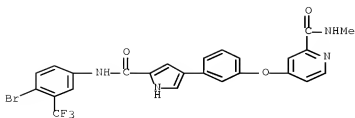
RN 852455-27-7 CAPLUS

CN 2-Pyridinecarboxamide, 4-[3-[5-[[4-chloro-2,5-dimethoxyphenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



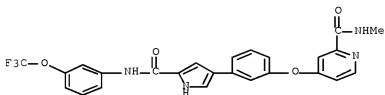
RN 852455-28-8 CAPLUS

CN 2-Pyridinecarboxamide, 4-[3-[5-[[4-bromo-3-(trifluoromethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



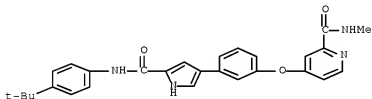
RN 852455-29-9 CAPLUS

CN 2-Pyridinecarboxamide, N-methyl-4-[3-[5-[[[3-(trifluoromethoxy)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl-2-pyridinecarboxamide (CA INDEX NAME)



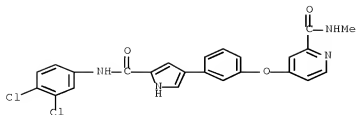
RN 852455-30-2 CAPLUS

CN 2-Pyridinecarboxamide, 4-[3-[5-[[[4-(1,1-dimethylethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl-2-pyridinecarboxamide (CA INDEX NAME)



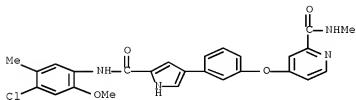
RN 852455-31-3 CAPLUS

CN 2-Pyridinecarboxamide, 4-[3-[5-[[[3,4-dichlorophenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl-2-pyridinecarboxamide (CA INDEX NAME)



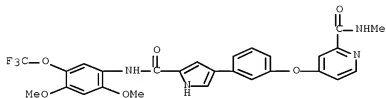
RN 852455-32-4 CAPLUS

CN 2-Pyridinecarboxamide, 4-[3-[5-[[4-chloro-2-methoxy-5-methylphenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



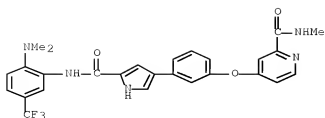
RN 852455-33-5 CAPLUS

CN 2-Pyridinecarboxamide, 4-[3-[5-[[[2,4-dimethoxy-5-(trifluoromethoxy)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



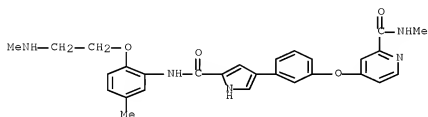
RN 852455-34-6 CAPLUS

CN 2-Pyridinecarboxamide, 4-[3-[5-[[[2-(dimethylamino)-5-(trifluoromethyl)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



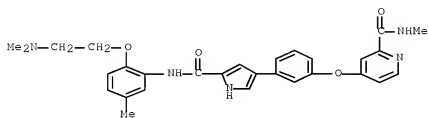
RN 852455-35-7 CAPLUS

CN 2-Pyridinecarboxamide, N-methyl-4-[3-[5-[[[5-methyl-2-(2-(methylamino)ethoxy)phenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]- (CA INDEX NAME)



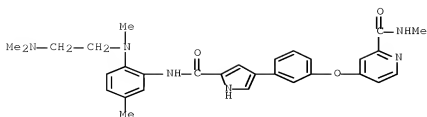
RN 852455-36-8 CAPLUS

CN 2-Pyridinecarboxamide, 4-[3-[5-[[[2-(2-(dimethylamino)ethoxy)-5-methylphenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



RN 852455-37-9 CAPLUS

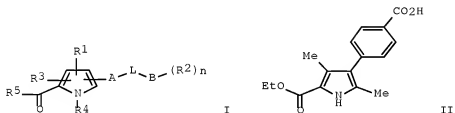
CN 2-Pyridinecarboxamide, 4-[3-[5-[[[2-[2-(dimethylamino)ethyl)methylamino]-5-methylphenyl]amino]carbonyl]-1H-pyrrol-3-yl]phenoxy]-N-methyl- (CA INDEX NAME)



L3 ANSWER 18 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:570508 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 141:106366
 TITLE: Preparation of substituted pyrroles as kinase inhibitors
 INVENTOR(S): Sun, Connie Li; Tang, Peng Cho; Ockey, Denise
 PATENT ASSIGNEE(S): Sugen, Inc., USA
 SOURCE: U.S. Pat. Appl. Publ., 44 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20040138269	A1	20040715	US 2003-679693	20031007
PRIORITY APPLN. INFO.:			US 2002-417555P	P 20021011
OTHER SOURCE(S):	MARPAT 141:106366			

GI



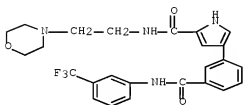
AB Title compds. I [R1 = H, alkyl, aryl, heteroaryl; R2 = alkyl, cycloalkyl, aryl, etc.; R3 = H, alkyl; R4 = H, alkyl, cycloalkyl, etc.; R5 = alkyl, cycloalkyl, aryl, heteroaryl, etc.; L = linker, e.g., alkyl-carboxamido, etc.; n = 0-5; A, B = cycloalkyl, aryl, heteroaryl] are prepared For instance, 3,5-dimethyl-1H-pyrrole-2-carboxylic acid Et ester is brominated in the 4-position (CH3CN, NBS, K2CO3) and coupled to 4-carboxyphenylboronic acid (DMF, (PPh3)4Pd, K2CO3, 18 h) to give II. I modulate the activity of protein kinases (PK) and are useful in treating disorders related to abnormal PK activity.

IT 720708-47-4P, 4-[3-(3-Trifluoromethylphenylcarbamoyl)phenyl]-1H-pyrrole-2-carboxylic acid [2-(morpholin-4-yl)ethyl]amide

720708-57-6P, 4-[4-[N'-(4-Isopropylphenyl)ureido]phenyl]-1H-pyrrole-2-carboxylic Acid [2-(morpholin-4-yl)ethyl]amide
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (substituted pyrroles as kinase inhibitors)

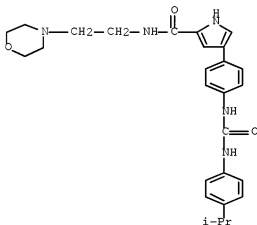
RN 720708-47-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[2-(4-morpholinyl)ethyl]-4-[3-[[[3-(trifluoromethyl)phenyl]amino]carbonyl]phenyl]- (CA INDEX NAME)



RN 720708-57-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[4-[[[4-(1-methylethyl)phenyl]amino]carbonyl]amino]phenyl]-N-[2-(4-morpholinyl)ethyl]- (CA INDEX NAME)



L3 ANSWER 19 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:292020 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 140:321233

TITLE: A preparation of pyrrole derivatives useful for the treatment of disorders ameliorated by reduction of TNF- α production and/or p38 activity

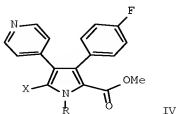
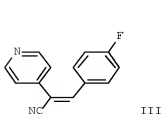
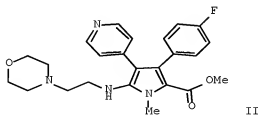
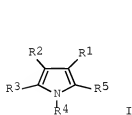
INVENTOR(S): Bullington, James L.; Fan, Xiaodong; Jackson, Paul F.; Zhang, Yue-mei

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

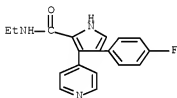
SOURCE: PCT Int. Appl., 116 pp.

DOCUMENT TYPE: CODEN: PIXXD2
 LANGUAGE: Patent
 FAMILY ACC. NUM. COUNT: English
 PATENT INFORMATION: 1

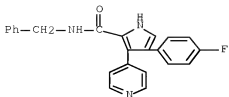
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004029040	A1	20040408	WO 2003-US30223	20030924
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2500221	A1	20040408	CA 2003-2500221	20030924
AU 2003278927	A1	20040419	AU 2003-278927	20030924
US 20050043331	A1	20050224	US 2003-670031	20030924
EP 1549635	A1	20050706	EP 2003-770442	20030924
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
BR 2003014783	A	20050726	BR 2003-14783	20030924
CN 1701069	A	20051123	CN 2003-825319	20030924
JP 2006511479	T	20060406	JP 2004-539896	20030924
MX 2005PA03264	A	20051018	MX 2005-PA3264	20050328
NO 2005001967	A	20050621	NO 2005-1967	20050422
ZA 2005003383	A	20060726	ZA 2005-3383	20050426
IN 2005KN00739	A	20060630	IN 2005-KN739	20050427
PRIORITY APPLN. INFO.:			US 2002-414436P	P 20020927
			WO 2003-US30223	W 20030924
OTHER SOURCE(S):		MARPAT 140:321233		
GI				



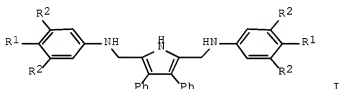
- AB The invention relates to 3-pyridyl-4-arylpyrrole derivs. of formula I [wherein: R1 and R2 are independently selected from (un)substituted (hetero)aryl; R3 = H, (un)substituted alkyl, -N:CR6-, -C(O)R7, etc.; R4 = H, (un)substituted alkyl, (un)substituted (hetero)aryl, etc.; R5 = (un)substituted alkyl, C(O)OR7, C(O)R7, CN, NO2, halo, etc.; R6 and R7 are independently selected from H, (un)substituted alkyl, (un)substituted aryl, (un)substituted heterocycle; with provisos], and pharmaceutical compns. comprising the same, useful for treating disorders ameliorated by reducing TNF- α production and/or p38 activity in appropriate cells. The invention compds. I were screened for p38 inhibition (in-vitro enzyme assays) and TNF- α inhibition (in-vitro whole cell assays and in vivo rodent assay). The invention also provides therapeutic and prophylactic methods using the instant pharmaceutical compns. For instance, pyrrole derivative II (compound 5; mouse 10 mg/kg, 0.5 h, 44% inhibition of TNF- α production) was prepared via condensation of 4-fluorobenzaldehyde with 4-pyridylacetonitrile, heterocyclization of the obtained pyridine derivative III with Me isocyanacetate, N-methylation of the pyrrole ring of the obtained pyrrolocarboxylate derivative IV (X = H, R = H), bromination of the pyrrolocarboxylate derivative IV (X = H, R = Me), and subsequent amination of the obtained bromopyrrole derivative IV (X = Br, R = Me) by 4-(2-aminoethyl)morpholine.
- IT 678161-63-2P 678161-84-7P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of pyridyl(aryl)pyrrole derivs. useful for the treatment of disorders ameliorated by reduction of TNF- α production and/or p38 activity)
- RN 678161-63-2 CAPLUS
- CN 1H-Pyrrole-2-carboxamide, N-ethyl-4-(4-fluorophenyl)-3-(4-pyridinyl)- (CA INDEX NAME)



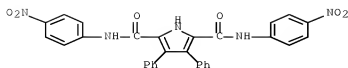
- RN 678161-84-7 CAPLUS
- CN 1H-Pyrrole-2-carboxamide, 4-(4-fluorophenyl)-N-(phenylmethyl)-3-(4-pyridinyl)- (CA INDEX NAME)



L3 ANSWER 20 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2003:290714 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 139:133415
 TITLE: Nitrophenyl derivatives of pyrrole 2,5-diamides:
 structural behavior, anion binding and color change
 signaled deprotonation
 AUTHOR(S): Camiolo, Salvatore; Gale, Philip A.; Hursthouse,
 Michael B.; Light, Mark E.
 CORPORATE SOURCE: School of Chemistry, University of Southampton,
 Southampton, SO17 1BJ, UK
 SOURCE: Organic & Biomolecular Chemistry (2003), 1(4), 741-744
 CODEN: OBCRAK; ISSN: 1477-0520
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:133415
 GI



AB Two new pyrrole 2,5-diamide clefts (I; R1 = NO2, R2 = H; R1 = H, R2 = NO2)
 have been synthesized. The 3,5-dinitrophenyl derivative has been shown to
 deprotonate in the presence of fluoride, which in acetonitrile solution, gives
 rise to a deep blue color.
 IT 566932-84-1P 566932-86-3P 566932-87-4P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and x-ray anal. of)
 RN 566932-84-1 CAPLUS
 CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-bis(4-nitrophenyl)-3,4-diphenyl- (CA
 INDEX NAME)



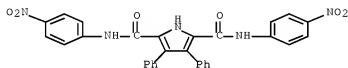
RN 566932-86-3 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxamide, N,N'-bis(4-nitrophenyl)-3,4-diphenyl-,
compd. with sulfinylbis[methane] (1:3) (9CI) (CA INDEX NAME)

CM 1

CRN 566932-84-1

CMF C30 H21 N5 O6



CM 2

CRN 67-68-5

CMF C2 H6 O S



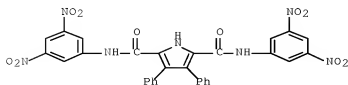
RN 566932-87-4 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxamide, N,N'-bis(3,5-dinitrophenyl)-3,4-diphenyl-,
compd. with sulfinylbis[methane] (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 566932-85-2

CMF C30 H19 N7 O10



CM 2

CRN 67-68-5

CMF C2 H6 O S

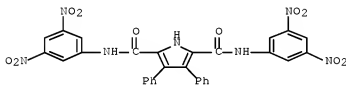


IT 566932-85-2E

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, x-ray anal., and chloride binding of)

RN 566932-85-2 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-bis(3,5-dinitrophenyl)-3,4-diphenyl-
(CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 21 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:276159 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:350593

TITLE: Crown Ether Appended Amidopyrrole Clefts

AUTHOR(S): Camiolo, Salvatore; Coles, Simon J.; Gale, Philip A.; Hursthouse, Michael B.; Tizzard, Graham J.

CORPORATE SOURCE: Department of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK

SOURCE: Supramolecular Chemistry (2003), 15(3), 231-234

CODEN: SCHEER; ISSN: 1061-0278

PUBLISHER: Taylor & Francis Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:350593

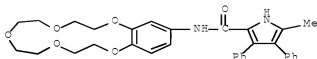
AB Two new pyrrole amide-crown ether conjugates have been synthesized and their anion complexation properties studied in the absence and presence of stoichiometric quantities of sodium or cesium cations. Certain anions are sequestered by the metal cation in DMSO-d₆ (0.5% water), however, in one case a 4.7 fold increase in the fluoride affinity of the receptor was observed upon addition of caesium cations. Crystal structure of one of the products was also reported.

IT 619326-15-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; preparation and crystal structure of crown
ether-appended amidopyrrole clefts and their anion complexation in
presence of sodium or cesium cations)

RN 619328-75-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 5-methyl-N-(2,3,5,6,8,9,11,12-octahydro-
1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)-3,4-diphenyl- (CA INDEX
NAME)



IT 619328-75-5DP, halide, benzoate, and phosphate complexes

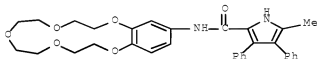
619328-76-6DP, halide, benzoate, and phosphate complexes

619328-76-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of crown ether-appended amidopyrrole clefts and their anion
complexation in presence of sodium or cesium cations)

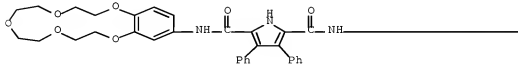
RN 619328-75-5 CAPLUS

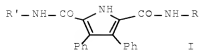
CN 1H-Pyrrole-2-carboxamide, 5-methyl-N-(2,3,5,6,8,9,11,12-octahydro-
1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)-3,4-diphenyl- (CA INDEX
NAME)



RN 619328-76-6 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-bis(2,3,5,6,8,9,11,12-octahydro-
1,4,7,10,13-benzopentaoxacyclopentadecin-15-yl)-3,4-diphenyl- (CA INDEX
NAME)





AB Four amido-pyrrole cleft anion receptors bearing one or two ferrocene reporter groups, e.g., I [R = R' = CH₂Fc 1, Fc 2; R = Ph, R' = CH₂Fc 3, Fc 4, Fc = (C₅H₅)₂Fe] were synthesized and crystallog. characterized. The receptors contain either a nonconjugated (1 and 3) or conjugated (2 and 4) link between the anion binding amido-pyrrole unit and the ferrocene reporter groups. The anion binding affinities and electrochem. behavior of the receptors in the absence and presence of anions were studied by ¹H NMR titration techniques and cyclic voltammetry using a Pt microdisc working electrode, resp.

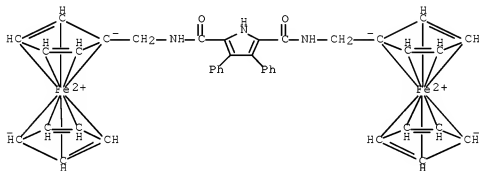
IT 475148-10-8P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(crystal structure, electrochem.; solid-state assembly, anion binding affinities and electrochem. properties of mono- and bis-ferrocene diamidopyrrole clefts)

RN 475148-10-8 CAPLUS

CN Ferrocene, 1,1'-(3,4-diphenyl-1H-pyrrole-2,5-diyl)bis(carbonyliminomethylene))bis- (9CI) (CA INDEX NAME)



IT 566915-30-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(crystal structure; preparation and amidation with aniline in the synthesis of mono- and bis-ferrocene diamidopyrrole clefts as electrochem. anion receptors)

RN 566915-30-8 CAPLUS

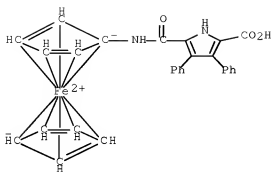
CN Ferrocene, [[5-carboxy-3,4-diphenyl-1H-pyrrol-2-yl]carbonyl]amino]-, compd. with trichloromethane (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 566915-29-5

CMF C28 H22 Fe N2 O3

CCI CCS



CM 2

CRN 67-66-3

CMF C H Cl3



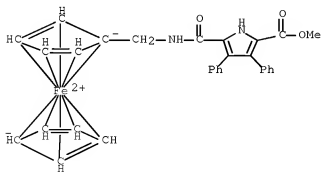
IT 566915-24-0P 566915-25-1P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(crystal structure; preparation and saponification in the synthesis of mono- and bis-ferrocene diamidopyrrole clefts as electrochem. anion receptors)

RN 566915-24-0 CAPLUS

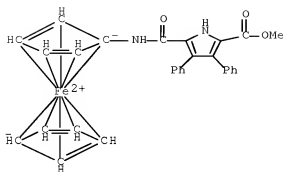
CN Ferrocene, [[[[5-(methoxycarbonyl)-3,4-diphenyl-1H-pyrrol-2-yl]carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)



RN 566915-25-1 CAPLUS

CN Ferrocene, [[[[5-(methoxycarbonyl)-3,4-diphenyl-1H-pyrrol-2-

yl]carbonyl]amino]- (9CI) (CA INDEX NAME)



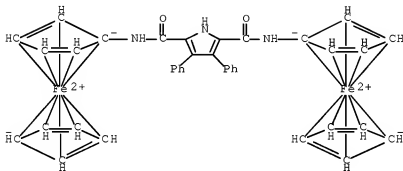
IT 475148-12-0P 566915-20-6P 566915-22-8P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(crystal structure; solid-state assembly, anion binding affinities and electrochem. properties of mono- and bis-ferrocene diamidopyrrole clefts)

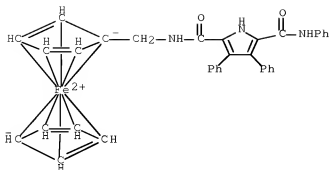
RN 475148-12-0 CAPLUS

CN Ferrocene, 1,1'-[(3,4-diphenyl-1H-pyrrole-2,5-diyl)bis(carbonylimino)]bis-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 566915-20-6 CAPLUS

CN Ferrocene, [[[(3,4-diphenyl-5-[(phenylamino)carbonyl]-1H-pyrrol-2-yl]carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)



RN 566915-22-8 CAPLUS

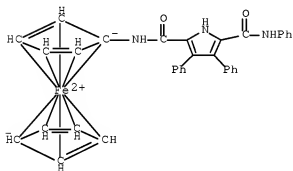
CN Ferrocene, [[3,4-diphenyl-5-[(phenylamino)carbonyl]-1H-pyrrol-2-yl]carbonyl]amino]-, compd. with methanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 566915-21-7

CMF C34 H27 Fe N3 O2

CCI CCS



CM 2

CRN 67-56-1

CMF C H4 O

H₃C-OH

IT 566915-29-5P

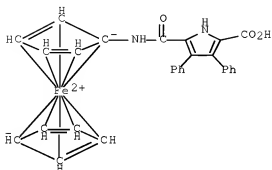
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(mol. structure; preparation and amidation with aniline in the synthesis of mono- and bis-ferrocene diamidopyrrole clefts as electrochem. anion

receptors)

RN 566915-29-5 CAPLUS

CN Ferrocene, [[(5-carboxy-3,4-diphenyl-1H-pyrrol-2-yl)carbonyl]amino]- (9CI)
(CA INDEX NAME)



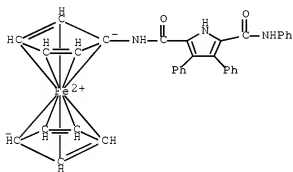
IT 566915-21-7P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(mol. structure; solid-state assembly, anion binding affinities and electrochem. properties of mono- and bis-ferrocene diamidopyrrole clefts)

RN 566915-21-7 CAPLUS

CN Ferrocene, [[[3,4-diphenyl-5-[(phenylamino)carbonyl]-1H-pyrrol-2-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)



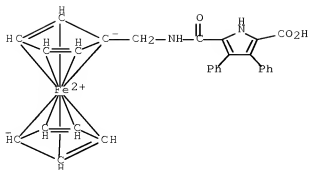
IT 566915-26-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and amidation with aniline in the synthesis of mono- and bis-ferrocene diamidopyrrole clefts as electrochem. anion receptors)

RN 566915-26-2 CAPLUS

CN Ferrocene, [[[5-carboxy-3,4-diphenyl-1H-pyrrol-2-yl]carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 23 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:689617 CAPLUS Full-text

DOCUMENT NUMBER: 138:62059

TITLE: Pendant arm pyrrolic amide cleft anion receptors

AUTHOR(S): Navakhun, Korakot; Gale, Philip A.; Camiolo, Salvatore; Light, Mark E.; Hursthouse, Michael B. Department of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2002), (18), 2084-2085

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The propensity of amine, ammonium and amide pendant arm 2,5-diamidopyrrole derivs. to act as anion receptors has been investigated. The anion-coordination ability of these species has been determined by 1H NMR titration techniques revealing a marked selectivity of the amine functionalized receptor for hydrogen sulfate anions.

IT 479401-36-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(X-ray structure of pendant arm pyrrolic amide cleft receptors)

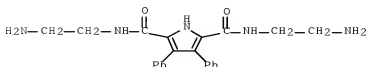
RN 479401-36-0 CAPLUS

CN Phosphate(1-), hexafluoro-, hydrogen, compd. with N,N'-bis(2-aminoethyl)-3,4-diphenyl-1H-pyrrole-2,5-dicarboxamide (1:1), dihydrate (9CI) (CA INDEX NAME)

CM 1

CRN 479401-33-7

CMF C22 H25 N5 O2



CM 2

CRN 16940-81-1

CMF F6 P . H

CCI CCS



IT 479401-34-8P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent) (pendant arm pyrrolic amide cleft anion receptors)

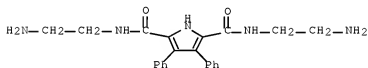
RN 479401-34-8 CAPLUS

CN Phosphate(1-), hexafluoro-, hydrogen, compd. with N,N'-bis(2-aminoethyl)-3,4-diphenyl-1H-pyrrole-2,5-dicarboxamide (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 479401-33-7

CMF C22 H25 N5 O2



CM 2

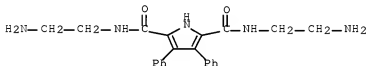
CRN 16940-81-1

CMF F6 P . H

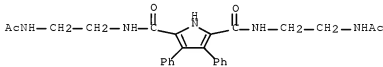
CCI CCS



IT 479401-33-7P 479401-35-9P
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
 (pendant arm pyrrolic amide cleft anion receptors)
 RN 479401-33-7 CAPLUS
 CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-bis(2-aminoethyl)-3,4-diphenyl- (CA INDEX NAME)



RN 479401-35-9 CAPLUS
 CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-bis[2-(acetylamino)ethyl]-3,4-diphenyl- (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 24 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2002:675089 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 138:122276
 TITLE: Confirmation of a cleft-mode' of binding in a 2,5-diamidopyrrole anion receptor in the solid state
 AUTHOR(S): Camiolo, Salvatore; Gale, Philip A.; Hursthouse, Michael B.; Light, Mark E.
 CORPORATE SOURCE: University of Southampton, Department of Chemistry, Southampton, SO17 1BJ, UK
 SOURCE: Tetrahedron Letters (2002), 43(39), 6995-6996

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The crystal structure of the tetrabutylammonium benzoate complex of 3,4-diphenyl-1H-pyrrole-2,5-dicarboxylic acid bis-butylamide has been elucidated confirming the formation of a cleft conformation in the solid state upon anion binding.

IT 468787-58-2

RL: PRP (Properties)

(crystal structure; crystal structure of tetrabutylammonium benzoate complex of diphenylpyrroledicarboxylic acid bis-butylamide)

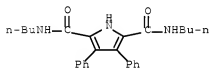
RN 488787-58-2 CAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, benzoate, compd. with
N,N'-dibutyl-3,4-diphenyl-1H-pyrrole-2,5-dicarboxamide (1:1) (9CI) (CA
INDEX NAME)

CM 1

CRN 365214-49-9

CMF C26 H31 N3 O2



CM 2

CRN 18819-89-1

CMF C16 H36 N . C7 H5 O2

CM 3

CRN 10549-76-5

CMF C16 H36 N



CM 4

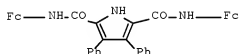
CRN 766-76-7

CMF C7 H5 O2

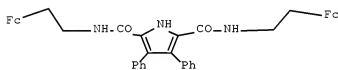


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 25 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2002:477989 CAPLUS Full-text
 DOCUMENT NUMBER: 137:370181
 TITLE: Anion complexation and electrochemical behavior of ferrocene-appended amido-pyrrole clefts
 AUTHOR(S): Denuault, Guy; Gale, Philip A.; Hursthouse, Michael B.; Light, Mark E.; Warriner, Colin N.
 CORPORATE SOURCE: Department of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
 SOURCE: New Journal of Chemistry (2002), 26(7), 811-813
 CODEN: NJCHE5; ISSN: 1144-0546
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 137:370181
 GI



I



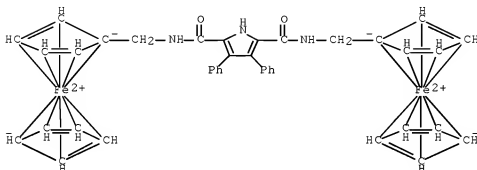
II

AB Two amido-pyrrole cleft anion receptors bearing two ferrocene reporter groups, e.g., I and II [Fc = (C5H4)Fe(C5H5)] were synthesized and crystallog. characterized; the receptors contain either a nonconjugated or conjugated link between the anion-binding amido-pyrrole unit and the ferrocene reporter groups. The anion binding affinities and electrochem. behavior of the receptors in the absence and presence of anions were studied by 1H NMR titration techniques and cyclic voltammetry using a Pt microdisc working electrode, resp.
 IT 475148-10-8P 475148-12-0P
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical

process); PRP (Properties); SPN (Synthetic preparation); PREP
(Preparation); PROC (Process)
(preparation, electrochem. and crystal structure of)

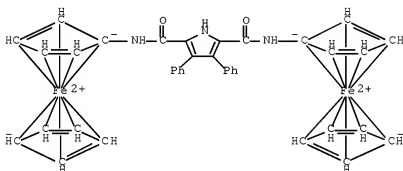
RN 475148-10-8 CAPLUS

CN Ferrocene, 1,1'-[(3,4-diphenyl-1H-pyrrole-2,5-
diyl)bis(carbonyliminomethylene)]bis- (9CI) (CA INDEX NAME)



RN 475148-12-0 CAPLUS

CN Ferrocene, 1,1'-[(3,4-diphenyl-1H-pyrrole-2,5-diyl)bis(carbonylimino)]bis-
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 26 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:219745 CAPLUS Full-text

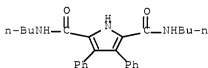
DOCUMENT NUMBER: 137:109012

TITLE: Solution and solid-state studies of
3,4-dichloro-2,5-diamidopyrroles: formation of an
unusual anionic narcissistic dimer

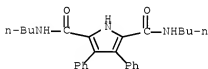
AUTHOR(S): Camilo, Salvatore; Gale, Philip A.; Hursthouse,
Michael B.; Light, Mark E.; Shi, Andy J.
CORPORATE SOURCE: Department of Chemistry, University of Southampton,
Southampton, SO17 1BJ, UK

SOURCE: Chemical Communications (Cambridge, United Kingdom)
(2002), (7), 758-759

CODEN: CHCOFS; ISSN: 1359-7345
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 137:109012
 AB 3,4-Dichloro-1H-pyrrole-2,5-dicarboxylic acid bis-phenylamide 3 and 3,4-dichloro-1H-pyrrole-2,5-dicarboxylic acid bis-butylamide 4 were prepared and shown to deprotonate in the presence of basic anions: the x-ray crystal structure of the tetrabutylammonium salt of 3-H⁺ reveals the formation of a dimer in the solid state.
 IT 365214-49-9
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
 (chloride receptor; solution and solid-state studies of unusual anionic narcissistic dimer of 3,4-dichloro-2,5-diamidopyrroles)
 RN 365214-49-9 CAPLUS
 CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-dibutyl-3,4-diphenyl- (CA INDEX NAME)



IT 443785-00-0
 RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
 (solution and solid-state studies of unusual anionic narcissistic dimer of 3,4-dichloro-2,5-diamidopyrroles)
 RN 443785-00-0 CAPLUS
 CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-dibutyl-3,4-diphenyl-, chloride (1:1) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 27 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2001:759709 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 136:37467
 TITLE: 2-Amidopyrroles and 2,5-Diamidopyrroles as Simple Anion Binding Agents
 AUTHOR(S): Gale, Philip A.; Camiolo, Salvatore; Tizzard, Graham J.; Chapman, Christopher P.; Light, Mark E.; Coles,

CORPORATE SOURCE: Simon J.; Hursthouse, Michael B.
 Department of Chemistry, University of Southampton,
 Southampton, SO17 1BJ, UK
 SOURCE: Journal of Organic Chemistry (2001), 66(23), 7849-7853
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:37467

AB Four new 2-pyrrolicarboxamides and 2,5-pyrroledicarboxamides have been synthesized and their anion complexation properties investigated. The crystal structures of these receptors have been elucidated and reveal hydrogen bonding in the solid state leading to dimer and network formation. Selectivity for oxo-anions has been demonstrated by ¹H NMR titration techniques; the 2,5-pyrroledicarboxamides are particularly selective for dihydrogen phosphate and benzoate over halide anions.

IT 380537-10-0 380537-11-1

RL: PRP (Properties)

(crystal structure; preparation, crystal structures, and anion complexation properties of pyrrolicarboxamides and pyrroledicarboxamides)

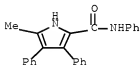
RN 380537-10-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 5-methyl-N,3,4-triphenyl-, compd. with dichloromethane (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 380537-09-7

CMF C24 H20 N2 O



CM 2

CRN 75-09-2

CMF C H2 Cl2

c1—CH2—c1

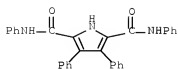
RN 380537-11-1 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxamide, N,N',3,4-tetraphenyl-, compd. with sulfinylbis[methane] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 365214-50-2

CMF C30 H23 N3 O2



CM 2

CRN 67-68-5

CMF C2 H6 O S

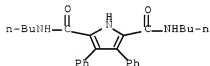


IT 365214-49-9P 365214-50-2P 380537-08-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; preparation, crystal structures, and anion complexation
properties of pyrrolicarboxamides and pyrroledicarboxamides)

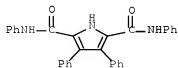
RN 365214-49-9 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-dibutyl-3,4-diphenyl- (CA INDEX NAME)



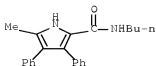
RN 365214-50-2 CAPLUS

CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5,3,4-tetraphenyl- (CA INDEX NAME)

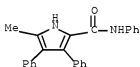


RN 380537-08-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-butyl-5-methyl-3,4-diphenyl- (CA INDEX NAME)

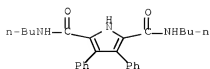


IT 360537-09-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation, crystal structures, and anion complexation properties of
 pyrrolicarboxamides and pyrrolicdicarboxamides)
 RN 380537-09-7 CAPLUS
 CN 1H-Pyrrole-2-carboxamide, 5-methyl-N,3,4-triphenyl- (CA INDEX NAME)

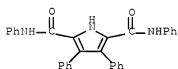


REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 28 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2001:498916 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 135:288487
 TITLE: Hydrogen-bonding pyrrolic amide cleft anion receptors
 AUTHOR(S): Gale, P. A.; Camiolo, S.; Chapman, C. P.; Light, M.
 E.; Hursthouse, M. B.
 CORPORATE SOURCE: Department of Chemistry, University of Southampton,
 Southampton, SO17 1BJ, UK
 SOURCE: Tetrahedron Letters (2001), 42(30), 5095-5097
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 135:288487
 AB The use of simple 2,5-diamidopyrrole derivs. as anion receptors has been
 investigated. Reaction of 3,4-diphenylpyrrole-2,5-dicarboxylic acid chloride
 with n-butylamine or aniline has produced two new amidic cleft anion receptors
 1 and 2. The anion-coordination ability of these species has been determined
 by 1H NMR titration techniques. Crystal structures of 1 and 2 have been
 elucidated, revealing a continuous hydrogen bonding network formed by 1 and
 dimerization of 2 via NH...O and CH...O hydrogen bonds.
 IT 365214-49-9 365214-50-2
 RL: PEP (Physical, engineering or chemical process); PRP (Properties);
 PROC (Process)
 (anion receptor; hydrogen-bonding pyrrolic amide cleft anion receptors)
 RN 365214-49-9 CAPLUS
 CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5-dibutyl-3,4-diphenyl- (CA INDEX NAME)

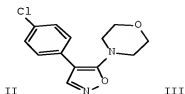
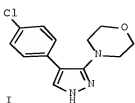
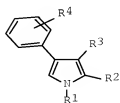


RN 365214-50-2 CAPLUS
 CN 1H-Pyrrole-2,5-dicarboxamide, N2,N5,3,4-tetraphenyl- (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 29 OF 43 CAPLUS COPYRIGHT 2008 ACS ON STN
 ACCESSION NUMBER: 1998:115 CAPLUS Full-text
 DOCUMENT NUMBER: 128:84047
 ORIGINAL REFERENCE NO.: 128:16249a,16252a
 TITLE: Synthesis, Anticonvulsant Activity, and Structure-Activity Relationships of Sodium Channel Blocking 3-Aminopyrroles
 AUTHOR(S): Unverferth, Klaus; Engel, Juergen; Hoefgen, Norbert; Rostock, Angelika; Guenther, Ralf; Lankau, Hans-Joachim; Menzer, Manfred; Rolfs, Andreas; Liebscher, Juergen; Mueller, Birgit; Hofmann, Hans-Joerg
 CORPORATE SOURCE: Corporate Research and Development ASTA Medica Group, Arzneimittelwerk Dresden GmbH, Radebeul, D-01445, Germany
 SOURCE: Journal of Medicinal Chemistry (1998), 41(1), 63-73
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

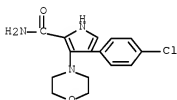


AB Starting from the corresponding acetophenone and glycine derivs., a series of new 3-aminopyrroles I [R1 = H, Me, PhCH2, Ac, PrCO, Bz, PhO2C, 4-morpholinylcarbonyl, EtSO2; R2 = CO2Me, CO2Et, CN, CO2CH2CHMe2, CO2H, H, CONH2, CONHPr, CONHCH2CH:CH2, CONHCH2CH2OMe, CONMe2, 4-morpholinylcarbonyl, 1-(4-methylpiperazinyl)carbonyl, COMe, CH2CH2CO2Me; R3 = 4-morpholinyl, NEt2, NMe2, 4-phenyl-1-piperazinyl, 4-methyl-1-piperazinyl, NMeCH2CH2NMe2; R4 = 4-Cl, 4-Br, 3-Br, 2-Me, H, 4-F, 4-Et] was synthesized in few steps. Using this procedure with hydrazine and hydroxylamine instead of the glycinates provides access to 3-aminopyrrole II and 5-amino-1,2-oxazole III. The various derivs. were tested for anticonvulsant activity in a variety of test models. Several compds. exhibit considerable activity with a remarkable lack of neurotoxicity. Ester I (R1 = H, R2 = CO2Me, R3 = 4-morpholinyl, R4 = 4-Br) (IV) was the most active compound. IV was protective in the maximal electroshock seizure (MES) test in rats with an oral ED50 of 2.5 mg/kg with no neurotoxicity noted at doses up to 500 mg/kg. IV blocks sodium channels in a frequency-dependent manner. The essential structural features which could be responsible for an interaction with an active site of the voltage-dependent sodium channel are established within a suggested pharmacophore model.

IT 183591-86-0P 200862-96-0P 200862-97-1F
200862-98-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, anticonvulsant activity, and structure-activity relationships of sodium channel blocking aminopyrroles)

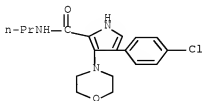
RN 183591-88-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-3-(4-morpholinyl)- (CA INDEX NAME)



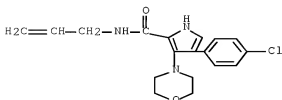
RN 200862-96-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-3-(4-morpholinyl)-N-propyl- (CA INDEX NAME)



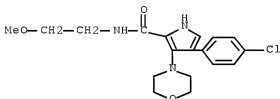
RN 200862-97-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-3-(4-morpholinyl)-N-2-propen-1-yl- (CA INDEX NAME)



RN 200862-98-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-N-(2-methoxyethyl)-3-(4-morpholinyl)- (CA INDEX NAME)



REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 30 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:120169 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 126:199420

ORIGINAL REFERENCE NO.: 126:38551a,38554a

TITLE: Mechanistic aspects of the synthesis of
3-aminopyrroles from substituted
2-methyl-1,2-thiazolium salts or
3-aminothioacrylamides. [Erratum to document cited in
CA126:7936]

AUTHOR(S): Rolfs, Andreas; Jones, Peter G.; Liebscher, Juergen
CORPORATE SOURCE: Inst. Chemie, Humboldt-Univ., Berlin, D-10115, Germany
SOURCE: Journal of the Chemical Society, Perkin Transactions
1: Organic and Bio-Organic Chemistry (1997), (2), 183

CODEN: JCPRB4; ISSN: 0300-922X
Royal Society of Chemistry

PUBLISHER: Journal

DOCUMENT TYPE: English

LANGUAGE: English

AB In Scheme 2, the structure for compound 6 is corrected The error was not reflected in the abstract or the index entries.

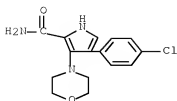
IT 183591-88-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrroles by ring transformation and desulfurization of
thiazolium compds. (Erratum))

RN 183591-88-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-3-(4-morpholinyl)- (CA INDEX

NAME)



L3 ANSWER 31 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:635701 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 126:7936

ORIGINAL REFERENCE NO.: 126:1767a,1770a

TITLE: Mechanistic aspects of the synthesis of
3-aminopyrroles from substituted
2-methyl-1,2-thiazolium salts or
3-aminothioacrylamides

AUTHOR(S): Rolfs, Andreas; Jones, Peter G.; Liebscher, Juergen
CORPORATE SOURCE: Inst. Chemie, Humboldt-Univ., Berlin, D-10115, Germany
SOURCE: Journal of the Chemical Society, Perkin Transactions
1: Organic and Bio-Organic Chemistry (1996), (19),
2339-2343

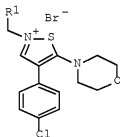
PUBLISHER: CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Royal Society of Chemistry

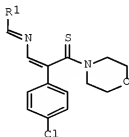
LANGUAGE: Journal

OTHER SOURCE(S): English

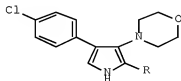
GI CASREACT 126:7936



I



II



III

AB The mechanism of the synthesis of 3-aminopyrrole derivs. by ring
transformation-desulfurization of substituted 2-methyl-1,2-thiazolium salts

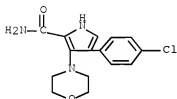
was investigated. The thiazolium salts I (R1 = 4-nitrophenyl, amido) were transformed into the thioamide derivs. II (same R1). II were subsequently transformed into the pyrroles III (R = cyano, amido).

IT 183591-88-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrroles by ring transformation and desulfurization of thiazolium compds.)

RN 183591-88-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(4-chlorophenyl)-3-(4-morpholinyl)- (CA INDEX NAME)



L3 ANSWER 32 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:994741 CAPLUS Full-text

DOCUMENT NUMBER: 124:86809

ORIGINAL REFERENCE NO.: 124:16315a,16318a

TITLE: Preparation of (pyrrolyl- and thienylcarbonyl)guanidines as sodium-hydrogen exchange inhibitors, antiarrhythmic agents, and cell proliferation inhibitors

INVENTOR(S): Kleemann, Heinz-Werner; Lang, Hans-Jochen; Schwark, Jan-Robert; Weichert, Andreas; Scholz, Wolfgang; Albus, Udo

PATENT ASSIGNEE(S): Hoechst A.-G., Germany

SOURCE: Eur. Pat. Appl., 48 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

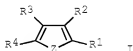
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 676395	A2	19951011	EP 1995-105088	19950405
EP 676395	A3	19960306		
EP 676395	B1	20030903		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
DE 4412334	A1	19951019	DE 1994-4412334	19940411
AT 248817	T	20030915	AT 1995-105088	19950405
ES 2206471	T3	20040516	ES 1995-105088	19950405
FI 9501681	A	19951012	FI 1995-1681	19950407
AU 9516354	A	19951019	AU 1995-16354	19950407
AU 683722	B2	19971120		
US 5698581	A	19971216	US 1995-418434	19950407
CA 2146707	A1	19951012	CA 1995-2146707	19950410
CA 2146707	C	20081021		
NO 9501405	A	19951012	NO 1995-1405	19950410

JP 07291927	A	19951107	JP 1995-107811	19950410
JP 4171078	B2	20081022		
ZA 9502930	A	19960126	ZA 1995-2930	19950410
HU 71616	A2	19960129	HU 1995-1035	19950410
CN 1117044	A	19960221	CN 1995-104391	19950410
CN 1073988	C	20011031		
IL 113310	A	20000629	IL 1995-113310	19950410
PRIORITY APPLN. INFO.:			DE 1994-4412334	A 19940411
OTHER SOURCE(S):		MARPAT 124:86809		
GI				

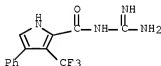


AB Title compds. [I; 1 of R1,R2 = CON:C(NH2)2 and the other = H, halo, alkyl, CON:C(NH2)2, NH2, etc.; R3,R4 = H, halo, cyano, alkyl, Ph, heteroaryl, etc.; Z = SOO-2, O, NR5; R5 = H, alkyl, etc.] were prepared Thus, Me 1-methylpyrrole-2-carboxylate was alkylated with (CF3)2CFI and the product amidated with guanidine to give I [R1 = CON:C(NH2)2, R2 = R3 = H, R4 = (CF3)2CF, Z = NMe] which ad IC50 of 0.3µM against Na+/H+ exchange in rabbit erythrocytes in vitro.

IT 172460-15-0P 172460-16-1P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of (pyrrolyl- and thienylcarbonyl)guanidines as sodium-hydrogen exchange inhibitors, antiarrhythmic agents, and cell proliferation inhibitors)

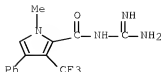
RN 172460-15-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-(aminoiminomethyl)-4-phenyl-3-(trifluoromethyl)- (CA INDEX NAME)



RN 172460-16-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-(aminoiminomethyl)-1-methyl-4-phenyl-3-(trifluoromethyl)- (CA INDEX NAME)



L3 ANSWER 33 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1995:218959 CAPLUS Full-text
 DOCUMENT NUMBER: 122:133846
 ORIGINAL REFERENCE NO.: 122:24979a,24982a
 TITLE: Preparation of small peptide anaphylatoxin receptor ligands
 INVENTOR(S): Or, Yat Sun; Luly, Jay R.
 PATENT ASSIGNEE(S): Abbott Laboratories, USA
 SOURCE: PCT Int. Appl., 58 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9407815	A2	19940414	WO 1993-US8173	19930830
W: CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRIORITY APPLN. INFO.:			US 1992-951684	A 19920925
OTHER SOURCE(S): MARPAT 122:133846				

AB Oligopeptide compds. or analogs represented by the formula A-B-D [A = R1-R2; B = R3-R4-R5; D = R6-R7-R8; R1 = H, alkyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, arylalkenyl, arylhydrazino, arylalkylamino, aminoalkyl, heterocyclyl, heterocyclylalkyl; R2 = CO, CS, CH2, SO2; provided that when R2 is CS or SO2, R1 may be H; R3, R6 = NR101 (wherein R101 = H, alkyl, arylalkyl); R4 = CR200R201, NR101, (E)- or (Z)-C:CHR205 (wherein R205 = arylalkyl); R5 = CO, CH2, CH2CO; R7 = CR210R211; R8 = H, CH2CO2H, CO2R100 (R100 = H, alkyl, arylalkyl); R200, R210 = H, alkyl, arylalkyl; R201 = (CH2)3Z (wherein Z = aryl or heterocyclyl attached to (CH2)3 through the ring C atom), CH2XCH2Z (wherein X = O, S, NH, alkylimino; Z = Z = aryl or heterocyclyl attached to CH2XCH2 through the ring C atom), CH2SCHR300W (wherein W = aryl; R300 = CO2H, alkoxycarbonyl, alkyl), CH2CH2XW (X, W = same as above), etc.; R211 = guanidinoalkyl; or R1R2 = H, alkyl, arylalkyl, aminoalkyl, guanidinoalkyl, provided that R1R2 is a group other than arylalkyl, R101 = arylalkyl; R1-R2-R3 = Q (wherein R' = H, alkyl); R1-R2-R3-R4 = arylalkylamino, heterocyclyl, arylalkyl, NHR50NR51 (wherein R50 = aroyl; R51 = aryl, arylalkyl)] are prepared These oligopeptides are ligands for the anaphylatoxin receptor and are useful for modulating C5a anaphylatoxin activity and in the treatment of inflammatory disease states. Thus, R-Arg(Tos)-Merrifield resin (I; R = Boc) was deprotected with 45% CF3CO2H in CH2Cl2 containing anisole and coupled with N-tert-butoxycarbonyl-(R)-2-amino-5-phenylpentanoic acid by using diisopropylcarbodiimide in CH2Cl2 and DMF to give I [R = (R)-2-amino-5-phenylpentanoyl] which was treated with HF(1) and anisole at 0° for 60 min to give N-[(R)-2-amino-5-phenylpentanoyl]-L-arginine. N-[(R)-2-(2-(indolecarbonylamino)-5-phenylpentanoyl)-L-arginine inhibited the binding of 125I-labeled C5a anaphylatoxin to purified PMNL membrane fragments with Ki of 0.56 μM.

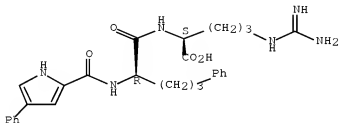
IT 159320-93-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as anaphylatoxin receptor ligand and antiinflammatory agent)

RN 159320-93-1 CAPLUS

CN L-Arginine, N2-[5-phenyl-N-[(4-phenyl-1H-pyrrol-2-yl)carbonyl]-D-norvalyl]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 34 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:511467 CAPLUS Full-text

DOCUMENT NUMBER: 117:111467

ORIGINAL REFERENCE NO.: 117:19447a,19450a

TITLE: Preparation of 3-aminopyrroles as analgesics and anticonvulsants

INVENTOR(S): Liebscher, Juergen; Knoll, A.; Ushmaev, A.; Rolfs, Andreas; Lohmann, Dieter; Faust, Gottfried;

PATENT ASSIGNEE(S): Morgenstern, Eveline; Scharfenberg, Peter
Arzneimittelwerk Dresden G.m.b.H., Germany
Ger. (East), 6 pp.

CODEN: GEXXA8

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

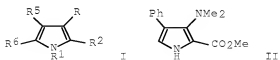
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 298915	A5	19920319	DD 1989-338226	19891117

PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 117:111467

GI



AB Title compds. {I; R = NR3R4; R1 = H, (cyclo)alkyl, arylalkyl, (hetero)aryl, CONH2, etc.; R2 = H, CHO, alkoxy carbonyl, CONH2, (hetero)aryl, cyano, NO2,

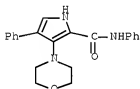
etc.; R3, R4 = H, (cyclo)alkyl, aralkyl, (hetero)aryl; NR3R4 = heterocyclyl; R5 = (hetero)aryl; R6 = H, alkyl, aryl, halo; R5R6 = alkylene] were prepared Thus, MeO2CCH2NHCH:CPHC(SMe):N+Me2 I- was cyclized to give title compound II which had ED50 of 4.5 + 10-5 mol/kg orally against maximal electroshock-induced convulsions in mice.

IT 135548-47-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as analgesic and anticonvulsant)

RN 135548-47-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-morpholinyl)-N,4-diphenyl- (CA INDEX NAME)



L3 ANSWER 35 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:490133 CAPLUS Full-text

DOCUMENT NUMBER: 117:90133

ORIGINAL REFERENCE NO.: 117:15733a,15736a

TITLE: Preparation aminopyrroles as analgesics and anticonvulsants

INVENTOR(S): Liebscher, Juergen; Knoll, A.; Ushmaev, A.; Rolfs, Andreas; Lohmann, Dieter; Faust, Gottfried; Morgenstern, Eveline; Scharfenberg, Peter
PATENT ASSIGNEE(S): Arzneimittelwerk Dresden G.m.b.H., Germany
SOURCE: Ger. (East), 7 pp.
CODEN: GEXXA8

DOCUMENT TYPE: Patent

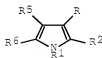
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

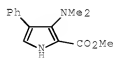
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 298914	A5	19920319	DD 1989-338219	19891117
PRIORITY APPLN. INFO.:			DD 1989-338219	19891117
OTHER SOURCE(S):	MARPAT	117:90133		

GI



I



II

AB The compds. [I; R = NR3R4; R1 = H, (cyclo)alkyl, aralkyl, (hetero)aryl, CONH2, etc.; R2 = H, CHO, alkoxy carbonyl, CONH2, (hetero)aryl, cyano, NO2, etc.; R3,

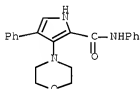
R4 = H, (cyclo)alkyl, aralkyl, (hetero)aryl; or NR3R4 = heterocyclyl; R5 = (hetero)aryl; R6 = H, alkyl, aryl, halo; or R5R6 = alkylene] were prepared. Thus Me2NCH:CHCSNMe2 was cyclocondensed with H2NCH2CO2Me to give title compound II which had ED50 of 4.5 ± 10^{-5} mol/kg p.o. for protection of mice against maximal electroshock-induced convulsions.

IT 135548-47-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, an analgesic and anticonvulsant)

RN 135548-47-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-morpholinyl)-N,4-diphenyl- (CA INDEX NAME)



L3 ANSWER 36 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:490132 CAPLUS Full-text

DOCUMENT NUMBER: 117:90132

ORIGINAL REFERENCE NO.: 117:15733a,15736a

TITLE: Preparation of 3-aminopyrroles as anticonvulsants and analgesics

INVENTOR(S): Liebscher, Juergen; Knoll, A.; Ushmaev, A.; Rolfs, Andreas; Lohmann, Dieter; Faust, Gottfried; Morgenstern, Eveline; Scharfenberg, Peter

PATENT ASSIGNEE(S): Arzneimittelwerk Dresden G.m.b.H., Germany

SOURCE: Ger. (East), 5 pp.

CODEN: GEXXA8

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 298918	A5	19920319	DD 1989-340208	19891117
PRIORITY APPLN. INFO.:			DD 1989-340208	19891117
OTHER SOURCE(S):		CASREACT 117:90132; MARPAT 117:90132		

GI



I



II

AB Title compds. [I; R = NR3R4; R1 = H, (cyclo)alkyl, aralkyl, (hetero)aryl, CONH2, etc.; R2 = H, CHO, alkoxycarbonyl, CONH2 (hetero)aryl cyano, NO2, etc.;

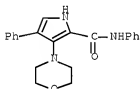
R3,R4 = H, (cyclo)alkyl, aralkyl, (hetero)aryl; NR3R4 = heterocyclyl; R5 = (hetero)aryl; R6 = H, alkyl, aryl, halo; R5R6 = alkylene] were prepared. Thus, pyrrole II (R = SH) was condensed with HNMe2 to give II (R = NMe2) which had ED50 of 4.5 + 10-5 mol/kg orally for protection of mice against maximal electroshock-induced convulsions.

IT 135548-47-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as analgesic and anticonvulsant)

RN 135548-47-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-morpholinyl)-N,4-diphenyl- (CA INDEX NAME)

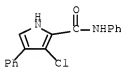


IT 142641-86-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of analgesics and anticonvulsants)

RN 142641-86-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-chloro-N,4-diphenyl- (CA INDEX NAME)



L3 ANSWER 37 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:469726 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 117:69726

ORIGINAL REFERENCE NO.: 117:12263a,12266a

TITLE: Process for preparation of 3-aminopyrrolecarboxylic acid derivatives as anticonvulsants and analgesics
INVENTOR(S): Liebscher, Juergen; Knoll, A.; Ushmaev, A.; Rolfs, Andreas; Lohmann, Dieter; Faust, Gottfried; Morgenstern, Eveline; Scharfenberg, Peter

PATENT ASSIGNEE(S): Arzneimittelwerk Dresden G.m.b.H., Germany
SOURCE: Ger. (East), 6 pp.

CODEN: GEXXA8

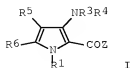
DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 298916	A5	19920319	DD 1989-340206	19891117



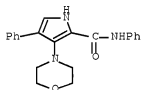
AB Nineteen title compds. I [R1 = H, (un)substituted alkyl, (un)substituted cycloalkyl, aralkyl, (un)substituted (hetero)aryl, acyl, alkoxycarbonyl, (un)substituted amino(thio)carbonyl; Z = OH, O-Metal, alkoxy, aryloxy, (un)substituted amino, alkylthio, arylthio; R3 = H, (un)substituted alkyl, cycloalkyl, aralkyl, (un)substituted (hetero)aryl; R4 = (un)substituted alkyl, cycloalkyl, aralkyl, (un)substituted (hetero)aryl; or R3R4 = alkylene optionally containing O, S, or N as a ring atom; R5 = (un)substituted (hetero)aryl; R6 = H, alkyl, aryl, halo; or R5R6 = alkylene] were prepared by standard functional transformations of the carboxylic acid moiety or its derived groups. For example, I [R1 = R6 = H, Z = OMe, R3R4 = (CH2)2O(CH2)2, R5 = 4-ClC6H4] (II) was prepared by standard direct esterification of the corresponding acid (Z = OH) using H2SO4 catalyst in refluxing MeOH (75% yield). II was slightly more potent than carbamazepine in the maximal electroconvulsion test in mice, and had a significantly higher protective index against neurotoxicity (36 vs. 5.1). General synthetic methods, addnl. biol. results, and capsule formulations are described.

IT 135548-47-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as anticonvulsant and analgesic)

RN 135548-47-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-morpholinyl)-N,4-diphenyl- (CA INDEX NAME)



L3 ANSWER 38 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:469725 CAPLUS Full-text

DOCUMENT NUMBER: 117:69725

ORIGINAL REFERENCE NO.: 117:12263a,12266a

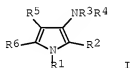
TITLE: Process for preparation of 2-substituted
3-aminopyrroles useful as anticonvulsives and
analgesics

INVENTOR(S): Liebscher, Juergen; Knoll, A.; Ushmaev, A.; Rolfs,
Andreas; Lohmann, Dieter; Faust, Gottfried;
Morgenstern, Eveline; Scharfenberg, Peter

PATENT ASSIGNEE(S): Arzneimittelwerk Dresden G.m.b.H., Germany
 SOURCE: Ger. (East), 6 pp.
 CODEN: GEXXA8
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 298917	A5	19920319	DD 1989-340207	19891117
PRIORITY APPLN. INFO.:			DD 1989-340207	19891117
OTHER SOURCE(S):		CASREACT 117:69725; MARPAT 117:69725		

GI



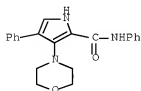
AB Nine title compds. I [R1 = H, (un)substituted alkyl, cycloalkyl, aralkyl, (hetero)aryl, acyl, alkoxy carbonyl, amino(thio)carbonyl; R2 = CHO, acyl, CO2H, alkoxy carbonyl, (un)substituted amino(thio)carbonyl, (hetero)aryl, NO2, cyano; R3 = H, (un)substituted alkyl, cycloalkyl, aralkyl, (hetero)aryl; R4 = (un)substituted alkyl, cycloalkyl, aralkyl, (hetero)aryl; or R3R4 = alkylene bridge optionally containing O, S, or N as ring atoms; R5 = (un)substituted (hetero)aryl; R6 = H, alkyl, aryl, halo; or R5R6 = alkylene bridge] were prepared by reaction of 2-unsubstituted I (R2 = H) with corresponding electrophiles, e.g., acid chlorides, anhydrides, or isocyanates. For example, I [R1 = R6 = H, R2 = CO2Me, R3R4 = (CH2)2O(CH2)2, R5 = Ph] (II) was prepared in 56% yield by acylation of the corresponding I (R2 = H) with ClCO2Me in refluxing MeCN. At 10-3 mol/kg orally in mice in the hot-plate test, II gave 90% inhibition, vs. 55% for analgin. General preps., addnl. biol. results, and capsule formulations are described.

IT 135548-47-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as anticonvulsive and analgesic)

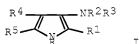
RN 135548-47-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-morpholinyl)-N,4-diphenyl- (CA INDEX NAME)



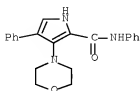
ACCESSION NUMBER: 1991:492063 CAPLUS Full-text
 DOCUMENT NUMBER: 115:92063
 ORIGINAL REFERENCE NO.: 115:15835a,15838a
 TITLE: Analgesic and anticonvulsant 3-aminopyrroles,
 INVENTOR(S): Liebscher, Juergen; Knoll, Alexander; Uschmajew,
 Alexej; Rolfs, Andreas; Lohmann, Dieter; Faust,
 Gottfried; Morgenstern, Eveline; Scharfenberg, Peter
 PATENT ASSIGNEE(S): Arzneimittelwerk Dresden G.m.b.H., Germany
 SOURCE: Eur. Pat. Appl., 27 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 431371	A1	19910612	EP 1990-121958	19901116
EP 431371	B1	19970910		
R: BE, CH, DE, ES, FR, GB, IT, LI, NL, SE				
DD 298912	A5	19920319	DD 1989-334670	19891117
SI 20323	A	20010228	SI 1990-12173	19901115
FI 9005689	A	19910518	FI 1990-5689	19901116
FI 102169	B	19981030		
FI 102169	B1	19981030		
HU 56343	A2	19910828	HU 1990-7176	19901116
JP 03271271	A	19911203	JP 1990-311258	19901116
JP 07113015	B	19951206		
US 5502051	A	19960326	US 1990-614459	19901116
RU 2060991	C1	19960527	RU 1990-4831894	19901116
ES 2108005	T3	19971216	ES 1990-121958	19901116
RU 2120796	C1	19981027	RU 1994-2476	19901116
US 5684160	A	19971104	US 1995-446000	19950519
PRIORITY APPLN. INFO.:			DD 1989-334670	A 19891117
			YU 1990-2173	A 19901115
			US 1990-614459	A3 19901116
OTHER SOURCE(S):		MARPAT 115:92063		
GI				

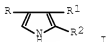


AB Aminopyrroles I [R = H, (un)substituted alkyl, cycloalkyl, aryl, heteroaryl, acyl, alkoxycarbonyl, carbamoyl, thiocarbamoyl; R1 = H, acyl, CO2H, alkoxycarbonyl, aryloxy carbonyl, carbamoyl, thiocarbamoyl, aryl, heteroaryl, cyano, NO2; R2, R3 = H, (un)substituted alkyl, cycloalkyl, aralkyl, aryl, heteroaryl; NR2R3 = heterocyclic; R4 = (un)substituted aryl, heteroaryl; R5 = H, alkyl, aryl, halogen; R4R5 = alkylene] were prepared by various methods. I (R = R5 = H, R1 = CO2Me, NR2R3 = morpholino, R4 = 4-ClC6H4), had an oral ED50 in the maximum electroshock test of 4.5 + 10⁻⁵ mg/kg. I (R = R5 = H, R1 = CO2H, CO2Me, NR2R3 = morpholino, R4 = Ph) caused 84.2 and 71.3% resp. inhibition of AcOH-induced writhing in mice.
 IT 135548-47-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)

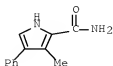
(preparation of)
 RN 135548-47-9 CAPLUS
 CN 1H-Pyrrole-2-carboxamide, 3-(4-morpholinyl)-N,4-diphenyl- (CA INDEX NAME)



L3 ANSWER 40 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1988:55811 CAPLUS Full-text
 DOCUMENT NUMBER: 108:55811
 ORIGINAL REFERENCE NO.: 108:9313a,9316a
 TITLE: A simple synthesis of pyrroles
 AUTHOR(S): Cohnen, Erich; Dewald, Renate
 CORPORATE SOURCE: Beiersdorf A.-G., Hamburg, D-2000/20, Fed. Rep. Ger.
 SOURCE: Synthesis (1987), (6), 566-8
 CODEN: SYNTBF; ISSN: 0039-7881
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 108:55811
 GI



AB Cyclocondensation of Me₂NCH:CRCOR¹ (R = CO₂Et, Ac, Bz, Ph, COCO₂Et; R¹ = Me, Et, Pr, Ph) with R³COCHR₂NH₂.HCl (R₂ = CONH₂, CN, Ac, CO₂Et; R₃ = NH₂, Me) gave 35-97% 16 pyrroles I.
 IT 112381-15-4P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and spectra of)
 RN 112381-15-4 CAPLUS
 CN 1H-Pyrrole-2-carboxamide, 3-methyl-4-phenyl- (CA INDEX NAME)



L3 ANSWER 41 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1971:448869 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 75:48869

ORIGINAL REFERENCE NO.: 75:7709a,7712a

TITLE: Independent syntheses of the products of acid- and base-catalyzed rearrangements of 2-(1-isoquinolyl)-3,3,5-triarylpyrrolenines

AUTHOR(S): McEwen, William E.; Berkebile, David H.; Liao, Tsung-Kai; Lin, Yun-Shan

CORPORATE SOURCE: Dep. Chem., Univ. Massachusetts, Amherst, MA, USA

SOURCE: Journal of Organic Chemistry (1971), 36(11), 1459-62
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

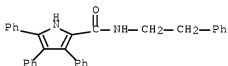
AB 2-(1-isoquinolyl)-3,4,5-triphenylpyrrole (I) and 2-(1-isoquinolyl)-3-p-anisyl-4,5-diphenylpyrrole (II) were synthesized by unambiguous methods. The synthetic samples are identical with the products of the acid- or base-catalyzed isomerization of 2-(1-isoquinolyl)-3,3,5-triphenylpyrrolenine (III) and the base-catalyzed isomerization of 2-(1-isoquinolyl)-3-p-anisyl-3,5-diphenylpyrrolenine (IV), resp. By inference, 2-(1-isoquinolyl)-4-p-anisyl-3,5-diphenylpyrrole (V) is the product of the acid-catalyzed isomerization of IV.

IT 28506-38-9P 28638-50-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

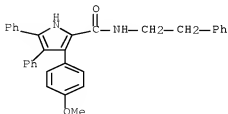
RN 28506-38-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 3,4,5-triphenyl-N-(2-phenylethyl)- (CA INDEX NAME)



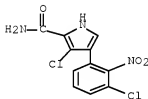
RN 28638-50-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-methoxyphenyl)-4,5-diphenyl-N-(2-phenylethyl)- (CA INDEX NAME)



L3 ANSWER 42 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1969:87561 CAPLUS Full-text
 DOCUMENT NUMBER: 70:87561
 ORIGINAL REFERENCE NO.: 70:16353a
 TITLE: 4-Phenylpyrrole-2-carboxylic amides
 INVENTOR(S): Hattori, Kiyoshi; Hashimoto, Masashi
 PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd.
 SOURCE: Jpn. Tokkyo Koho, 2 pp.
 CODEN: JAXXAD
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 44001528	B4	19690123	JP	19660721
AB	Manufacture of 3-chloro-4-(2-nitro-3-chlorophenyl)pyrrole-2-carboxamide (I), useful as a muscle relaxant, is described. Thus, 320 mg. 3-chloro-4-(2-nitro-3-chlorophenyl)pyrrole-2-carbonitrile is stirred with 7 cc. Me2CO, 250 mg. NaOH, and 3 cc. H2O, then stirred 30 min. more with 0.5 cc. 30% H2O2, let stand overnight with 1 cc. H2O, concentrated in vacuo, 10 cc. H2O added, and the precipitate recrystd. (AcOEt-C6H6) to give 76 mg. I, m. 202-3°.				
IT	21765-13-9P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)				
RN	21765-13-9 CAPLUS				
CN	1H-Pyrrole-2-carboxamide, 3-chloro-4-(3-chloro-2-nitrophenyl)- (CA INDEX NAME)				



L3 ANSWER 43 OF 43 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1961:144086 CAPLUS Full-text
 DOCUMENT NUMBER: 55:144086
 ORIGINAL REFERENCE NO.: 55:27263f-i, 27264a-i, 27265a-i, 27266a-e
 TITLE: A new route to the synthesis of the pyrrole ring system
 AUTHOR(S): Dimroth, Karl; Pintschovius, Ulrich
 CORPORATE SOURCE: Univ. Marburg, Germany
 SOURCE: Justus Liebig's Annalen der Chemie (1961), 639, 102-24
 CODEN: JLACBF; ISSN: 0075-4617
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 OTHER SOURCE(S): CASREACT 55:144086
 GI For diagram(s), see printed CA Issue.

AB N-Alkyl, N-aryl, or N-acylamines, containing in α, α' -positions 2 CH₂ groups activated by carbalkoxy or nitrile groups, condensed with Bz₂ in the presence of Me₃COK in 60-80% yields to 1-alkyl(aryl or acyl)-3,4-diphenylpyrrole derivs. bearing in the 2- and 5-positions CO₂H, carbalkoxy, CN, or carboxamide groups. The free pyrrole- α -carboxylic acids were readily decarboxylated by acids to the α, α' -unsubstituted pyrroles. The 1-acylpyrroles were hydrolyzed by bases to the pyrroles. The preparation of suitable CH₂-containing amine components was described. A simple cyanomethylation procedure with polyoxymethylene (I), KCN, and AcOH was described for the conversion of aromatic amines to the previously unknown bis(cyanomethyl) derivs. Crude PhN(CH₂CO₂H)₂ (55 g.), 250 cc. MeOH, and 20 cc. concentrated H₂SO₄ refluxed 7 hrs., concentrated in vacuo, diluted with iced H₂O, and extracted with Et₂O gave 73% PhN(CH₂CO₂Me)₂ (II), b₁₀ 183°, m. 47-9°. Similarly prepared was PhN(CH₂CO₂Et)₂, b₁₀ 188°. p-MeOC₆H₄NH₂, 1 mole ClCH₂CO₂H, and 1.5 moles NaOAc.3H₂O were converted to p-MeOC₆H₄NHCH₂CO₂H, which, heated 5 hrs. with 2.5 moles ClCH₂CO₂Na on the steam bath and then esterified in the usual manner with MeOH-H₂SO₄, gave p-MeOC₆H₄N(CH₂CO₂Me)₂ (III), b₁₁ 209°; III.HCl, m. 136-7° (absolute MeOH). p-MeC₆H₄NH₂ was converted similarly to p-MeC₆H₄N(CH₂CO₂Me)₂ (IV), b₁₀ 186°, m. 44.5-45°. p-ClC₆H₄NHCH₂CO₂H (40 g.) in dilute aqueous solution of 8.7 g. NaOH treated below 35° with a solution of 70 g. Cl-CH₂CO₂H and 30 g. NaOH (total volume of mixture about 500 cc.), heated 4-5 hrs. on the water bath, cooled, and filtered, and the residue treated with 80 cc. 6N HCl gave p-ClC₆H₄N(CH₂CO₂Me)₂ (V), b₁₀ 202-3°, m. 58-9°. p-H₂NC₆H₄CO₂H (13.7 g.) and 4 g. NaOH in H₂O treated with aqueous ClCH₂CO₂Na from 28.5 g. ClCH₂CO₂H, heated 8 hrs. on the water bath, cooled, and filtered, and the residue treated with HCl gave 54% p-HO₂CC₆H₄N(CH₂CO₂H)₂ (VI), decomposing 260°. VI (15 g.), 50 cc. MeOH, and 6 cc. H₂SO₄ heated 7 hrs. on the water bath gave 14.8 g. p-MeO₂CC₆H₄N(CH₂CO₂Me)₂ (VII), m. 91-2° (EtOH or ligroine); VII.HCl decomposing 85-90°. II in CCl₄ or AcOH treated with the calculated amount of Br at room temperature gave p-BrC₆H₄N(CH₂CO₂-Me)₂ (VIII), m. 64-6°, b₁₀ 216°; VII. H Br decomposing 130-1° (MeCN or EtOMe). II (10 g.) in 100 cc. AcOH treated with stirring and cooling with 3.3 cc. colorless 100% HNO₃ and poured after a few min. onto ice yielded 75-80% (crude) p-O₂NC₆H₄N(CH₂CO₂Me)₂ (VIII), yellow-brown needles with a bluish luster, m. 123-3.5° (CCl₄ or MeOH). Similarly prepared was p-O₂NC₆H₄N(CH₂CO₂Et)₂ (IX), 87%. m. 137°, which (hydrolyzed with alkali) gave p-O₂NC₆H₄N(CH₂CO₂H)₂, decomposing 202-5°. VIII reduced with Na₂S₂O₄ in aqueous EtOH and extracted with CHCl₃ gave p-H₂NC₆H₄N(CH₂CO₂Me)₂, m. 53-5°, b_{0.01} 156-9°; HCl salt decomposing 205-6°. NaHSO₃ (208 g.) in a min. of H₂O treated with 150 cc. 40% aqueous CH₂O, the mixture treated after 20 min. with stirring with 100 g. 30% aqueous MeNH₂, heated 20 min. on the water bath, treated with 134 g. KCN in 250 cc. H₂O, saturated with NaCl, and extracted with Et₂O yielded 48% MeN(CH₂CN)₂ (X), b₁₁ 130°; X.HCl decomposing 120-2°. p-O₂NC₆H₄NMe₂ (33 g.), 18.7 cc. 38% CH₂O, and 26 g. NaHSO₃ heated 15 min. at 100° with occasional shaking and treated with 16.5 g. KCN in 30 cc. H₂O yielded 31.5 g. crude p-Me₂NC₆H₄N(CH₂CN)₂Me (XI), m. 80°. Powdered KCN (8 g.), 14 g. XI, and 2.8 g. I treated with cooling with 65 cc. AcOH, heated 1 hr. at 50°, stirred several hrs., and poured into iced H₂O gave 13.6 g. p-Me₂NC₆H₄N(CH₂CN)₂ (XII), m. 127-8.5° (BuOH-EtOH); XII.HCl decomposing 207-10° (85% EtOH). NaHSO₃ (35 g.) and 25 cc. 38% aqueous CH₂O treated on the water bath with 41 g. p-MeOC₆H₄NH₂ and then with 22 g. KCN in 50 cc. H₂O and heated 20 min. on the water bath gave 42 g. p-MeOC₆H₄NHCH₂CN (XIII), m. 75-6° (MeOH or CCl₄). XIII (15.2 g.), 8.5 g. KCN, and 3.8 g. I treated dropwise with stirring and cooling with 100 cc. AcOH containing 3 drops concentrated H₂SO₄, heated 4 hrs. at 40-50°, and kept overnight yielded 18.3 g. p-MeOC₆H₄N(CH₂CN)₂ (XIV), m. 114-15°, b₉ 221.5°. PhNHCH₂CN (26.4 g.), b₁₁ 63°, with 17 g. KCN, 7.6 g. I, and 150 cc. AcOH gave 80% (crude) PhN(CH₂CN)₂ (XV), leaflets, m. 139-40° (BuOH). II with absolute EtOH and NH₃ gave PhN(CH₂CONH₂)₂ (XVI). XVI (10 g.) in 25 cc. Decalin heated 0.5 hr. at 180° with 10 g. P₂O₅ and extracted with C₆H₆ gave some XV; the mother liquor

yielded 4-phenyl-2,6-piperazinedione. m. 159-60°. p-MeC6H4NHCH2CN (20.5 g.), 11.5 g. KCN, 5.3 g. I. and 100 cc. AcOH gave 88% p-MeC6H4N(CH2CN)2, m. 119-20° (MeOH), b11 207°. p-MeC6H4NHCH2CO2Me (27 g.) (from 10 g. p-MeC6H4NH2 and 5.1 g. ClCH2CO2Me, m. 84-6°, 12.5 g. KCN, 6 g. I, and 100 cc. AcOH kept at 35° and then heated 2 hrs. at 50° gave 32.1 g. p-MeC6H4N-(CH2CN)CH2CO2Me (XVII), b10 195-5.5°, m. 80-1°. p-MeC6H4NHCH2Bz (14 g.) with 5 g. KCN, 2.3 g. I, and 60 cc. AcOH yielded (at 40°) p-MeC6H4N(CH2CN)CH2Bz, greenish crystals, m. 153-4.5°. PhNH2 (9.3 g.) and 35.2 g. iso-Pr2NEt treated at 0° with stirring with 40 g. BzCH2Br in 40 cc. CHCl3 and the mixture refluxed 0.5 hr., cooled, and filtered yielded 17.7 g. PhN(CH2Bz)2 (XVIII), m. 225-8° (MeOCH2CH2OH). BzCH2NHPh (26 g.) with 28.2 g. BzCH2Br and 17 g. iso-Pr2NEt refluxed in 40 cc. CHCl3 gave XVIII. III (2.7 g.) and 1.5 g. (CO2Et)2 (XIX) treated with 0.9 g. Na in 20 cc. MeOH, kept several days, warmed, and filtered, and the residue treated with HCl gave 1-(p-methoxyphenyl)-3,4-dihydropyrrole-2,5-dicarboxylic acid di-Me ester (XX), m. 185-8° (with gas evolution) (MeOCH2-CH2OH and EtCOMe). IX (4.0 g.) and 2.2 g. XIX in 60 cc. Me3COH treated at 50° with 1.2 g. K in 40 cc. Me3COH, kept 15 hrs., and evapd, in vacuo, and the residue extracted with MeOH gave 1-(p-nitrophenyl)-3,4-dihydropyrrole-2,5-dicarboxylic acid di-tert-Bu ester, m. 176-8° (AcOH, EtOH, and ligroine); it gave a green FeCl3 reaction. BzH (5 cc.) and 5 g. II in 20 cc. MeOH added dropwise at 2-5° to 2 g. Na in 30 cc. absolute MeOH, kept 2 hrs. at 0°, evaporated in vacuo below 30°, treated with cold HCl, and extracted with MeOH yielded 1.5 g. PhN[C(CHPh)CO2H]2, greenish yellow crystals, m. 161-3°; the mother liquor gave PhCH=C.NPh.CH2.CHPh.O.CO, m. 223-5° (decomposition) (85% AcOH); the filtrate diluted with CH2Cl2 precipitated a Na salt, which (trituated with concentrated HCl) gave BzCO2H, m. 14750°; it gave a dark green FeCl3 reaction. The filtrate from the BzCO2H treated with Br gave 2,4-Bz2C6H3NHCH2CO2H, prisms, m. 161° (petr. ether). Bz2 (5.3 g.) and 6.0 g. II in 30 cc. dry Et2O added dropwise with cooling and stirring to 4 g. K in 60 cc. absolute Me3COH and 20 cc. dry Et2O, the mixture kept 20 hrs. and evaporated below 40° in vacuo, and the residue treated with a small amount of H2O gave 1.3 g. yellow K salt (yellow in concentrated H2SO4), which (recrystd. from AcOH with heating) gave 1,3,4-triphenylpyrrole, needles, m. 150-7°, intense orange in concentrated H3SO4; it coupled with diazonium salts in AcOH. III (10 g.), 7.0 g. Bz2 in 50 cc. Et2O, and 5 g. K in 90 cc. Me3COH gave (in the usual manner during 20 min.) the 2-CO2Me derivative (XXI) of 1-(p-methoxyphenyl)-3,4-diphenylpyrrole (XXII), m. 169.5-71° (iso-AmOAc), and from the mother liquor the 2-CO2CMe3 derivative (XXIII) of XXII, needles, m. 128-9° (absolute EtOH). XXI refluxed 4 hrs. with 10% alc. KOH gave the carboxylic acid, m. about 200°, which (heated with a little H2SO4) gave XXII, prisms, m. 109-10° (EtOH). XXIII refluxed 5 hrs. with 5 drops concentrated HCl in 25 cc. EtOH gave also XII. IV (6.0 g.), 5.0 g. Bz2, and 4 g. K in 90 cc. Me3COH and 20 cc. Et2O neutralized after 4 hrs. with HCl, filtered, and evaporated gave 6 g. (crude) 1-(p-MeC6H4) analog (XXIV) of XXI, prisms, m. 130.5-31° (5:1 MeOH-C6H6). XXIV refluxed 4 hrs. with alc. KOH and decarboxylated with concentrated H2SO4 yielded the 2-CO2H derivative (XXV) of 1-(p-MeC6H4) analog (XXV) of XXII, m. 179-82°, which, recrystd. from AcOH and ligroine, yielded XXV, leaflets, m. 130-1° (AcOH-ligroine). Bz2 (5 g.) and 6.7 g. V condensed in the usual manner, treated after 4 hrs. with 10 cc. concentrated HCl, filtered, and kept some time at room temperature deposited 2.3 g. 1-(p-ClC6H4) analog (XXVI) of XX, m. 204.5-205°, with gas evolution (BuOH-EtOH and MeNO2), yellow in concentrated H2SO4; the mother liquor evaporated gave the p-ClC6H4 analog (XXVII) of XXI, prisms, m. 118-20° (EtOH and AcOH). XXVI and XXVII saponified with alkali and decarboxylated gave the 1-(p-ClC6H4) analog of XXII, m. 145-6° (AcOH or EtOH). K (3.8 g.) in 70 cc. Me3COH, 4.6 g. Bz2 in 20 cc. Et2O, and 7.6 g. VII in 30 cc. Me3COH heated 3 hrs., neutralized with HCl, and filtered, and the filtrate concentrated gave 3.0 g. (crude) 1-(p-BrC6H4) analog (XXVIII) of XX, prisms, m. 190-1° (3:1 BuOH-EtOH). XXVIII saponified with alkali and heated with H2SO4 gave the 1-(p-BrC6H4) analog of XXII, m. 135-7° (ligroine and AcOH). VI (5.5 g.) and 4.5 g. Bz2 in 160 cc. Et2O

treated 20 min. at 5° with 7.4 g. K in 85 cc. Me₃COH, the mixture evaporated in vacuo, adjusted with HCl to pH 8, and filtered, and the resinous residue (10 g.) refluxed 2 hrs. with alc. KOH, acidified, and ground with AcOH gave 1.6 g. 1-(p-HO₂CC₆H₄) analog of XXII, m. 241-3°, with browning (AcOH and AmOAc), yellow in concentrated H₂SO₄. VIII (7 g.), 5 g. Bz₂, and 3.8 g. K in 65 cc. Me₃COH, 90 cc. Et₂O, and 70 cc. dioxane kept 1 hr. at 5°, treated with 5 cc. AcOH, and evaporated, the residue washed with H₂O and dissolved in CHCl₃, and the CHCl₃ solution washed with aqueous NaHCO₃ (to remove about 0.6 g. organic acid) and evaporated gave a substance, m. 211-13° (light red in concentrated H₂SO₄), which could not be eluted from Al₂O₃ when chromatographed; the mother liquor chromatographed twice on Al₂O₃ gave the 1-(p-O₂NC₆H₄) analog (XXIX) of XXI, m. 193-5° (EtCOMe, AcOH, BuOH), intense orange-yellow in concentrated H₂SO₄; it gave a red dye with diazonium salts. K (3.4 g.) in 70 cc. Me₃COH, 5 g. XIV, and 5 g. Bz₂ in dioxane-Me₃COH treated with AcOH, evaporated in vacuo, and extracted with H₂O left 9.8 g. 1-(p-methoxyphenyl)-3,4-diphenyl-2-cyanopyrrole-5-carboxamide (XXX), prisms, m. 248.5-49° (BuOH). XVII (5.5 g.), 3.5 g. K in 100 cc. Me₃COH, and 5.3 g. Bz₂ in 50 cc. Me₃COH and 7 cc. dioxane treated with AcOH yielded similarly 8.2 g. 2-CN derivative of XXV, m. 142-2.7° (AcOH and ligroine). XII (4.3 g.) condensed during 2 hrs. with 4.2 g. Bz₂ and 3.4 g. K in 50 cc. Me₃COH and 50 cc. dioxane and evaporated, and the residue ground with warm MeOH and diluted with C₆H₆ precipitated the 1-(p-Me₂NC₆H₄) analog (XXXI) of XXX, m. 283°, with browning at 270° (HCONH₂); the mother liquor gave 1-(p-dimethylaminophenyl)-3,4-dihydroxy-3,4-diphenyl-2,5-dicyanopyrrolidine (XXXII), m. 221-3° (decomposition), which (triturated with 33% HCl) gave XXXII.HCl. K (4 g.) in 65 cc. Me₃COH condensed at 0° with 3.3 g. X and 6.3 g. Bz₂ in 75 cc. Et₂O, the mixture kept overnight and filtered, and the residue triturated with 80% AcOH gave 6 g. 1-Me analog of XXX, m. 276° colorless in concentrated H₂SO₄; the mother liquor gave a small amount of 1-methyl-3,4-diphenyl-2,5-dicyanopyrrole, m. 159-61° (90% EtOH). K (4 g.) in 85 cc. Me₃COH and 10 cc. Et₂O condensed with 5.25 g. Bz₂ and 7 g. AcN(CH₂CO₂Me)₂, m. 83.5-84°, b₁₅ 184°, in 40 cc. Me₃COH and 15 cc. dioxane, the mixture evaporated, washed with Et₂O, dissolved in H₂O, and acidified with HCl gave 1-acetyl-3,4-diphenylpyrrole-2,5-dicarboxylic acid (XXXIII), m. 254-5° (decomposition) (aqueous MeOH); the Et₂O-insol. residue chromatographed gave the Me ester (XXXIV) of XXXIII, m. 143-4° (MeOH). The residue from the Et₂O washing (4.6 g.) ground with MeOH and recrystd. repeatedly from PhMe-ligroine gave 3,4-diphenylpyrrole-2-carboxylic acid tert-Bu ester, leaflets, m. 164-5°, yellow in H₂SO₄. XXXIV refluxed 3 hrs. with 1.3 g. KOH in 20 cc. EtOH gave 3,4-diphenylpyrrole-2-carboxylic acid, m. 205-7°. BzN(CH₂CN)₂ (4 g.), m. 131-2°, and 4.1 g. Bz₂ in 40 cc. dry tetrahydrofuran and 35 cc. dry MeCN treated 1.5 hrs. with 1.6 g. K in 40 cc. Me₃COH and 50 cc. dry C₆H₆, stirred 3.5 hrs. at 20°, treated with 3.4 g. AcOH, filtered, and concentrated in vacuo to 1/3 volume yielded 1.3 g. 1-Bz analog (XXXV) of XXX, m. 239-41° (decomposition) (EtOH and iso-PrOH); the concentrated filtrate from the crude product diluted with Et₂O gave 3,4-diphenyl-2-cyanopyrrole-5-carboxamide (XXXVI), m. 294-7° (decomposition) (iso-Am₂O and MeOH). XXXV refluxed 8 hrs. with 4% alc. KOH gave 1.15 g. XXXVI, needles, m. 299-300° (MeCN-iso-PrOH). K (6.3 g.) in 100 cc. Me₃COH added to 9 g. acenaphthenequinone and 10 g. II in 50 cc. dry C₆H₆, refluxed 0.5 hr. and evaporated in vacuo, the residue extracted with Na₂CO₃, and the extract acidified carefully precipitated a mono-Na salt, which (with HCl) yielded 1.2 g. 1-phenyl-3,4-dihydroxy-3,4-(1,8-naphthylene)pyrrolidine-2,5-dicarboxylic acid, decomposing 221-2° (AcOH and 1:1 aqueous Me₂CO). XXXII (7 g.) in 100 cc. dry dioxane with 4.5 g. Bz₂ and 2.2 g. K in 40 cc. Me₃COH heated 5 hrs. at 35°, adjusted with HCl to pH 5, and filtered, and the filtrate evaporated gave about 1 g. 1-phenyl-2,5-dibenzoyl-3,4-dihydroxy-3,4-diphenylpyrrolidine, yellowish needles, decomposing 221-4° (Et₂CO), pale red in warm concentrated H₂SO₄. The infrared absorption spectra of XII, XXXI, and XXXII were recorded.

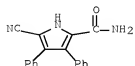
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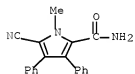
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CN 1H-Pyrrole-2-carboxamide, 5-cyano-3,4-diphenyl- (CA INDEX NAME)



RN 101895-84-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 5-cyano-1-methyl-3,4-diphenyl- (CA INDEX NAME)



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